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THEORETICAL GUN PROPELLANT THERMOCHEMICAL EVALUATION

GUNS AND ROCKETS BRANCH
ADVANCED DEVELOPMENT DIVISION

TECHNICAL REPORT AFATL-TR-71-11

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13 ABSTRACT

A computer program is presented for the computation of chemical equilibrium reaction products associated with gun propellant combustion. The program as developed at the Air Force Armament Laboratory was based on a code used by the NASA Lewis Research Center. The program provides a first approximation of flame temperature, specific heat ratio, impetus, and mean molecular weight of the combustion products. A simplified users manual is presented for thermochemical programs and for the program to generate specific heat polynomials from JANAF tabular data.

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Theoretical Gun Propellant Thermochemical Evaluation

Otto K. Heiney

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FOREWORD

This report has been generated under the advanced gun propellant evaluation analysis portion of Project 62602F 2560 and is presented as a state of the art advancement that can be applied to gun propellant research efforts. The study was conducted during the period February 1970 to January 1971.

This technical report has been reviewed and is approved.

Charles Petrides
CHARLES PETRIDES
Chief, Advanced Development Division

ABSTRACT

A computer program is presented for computing the chemical equilibrium reaction products associated with gun propellant combustion. This program will provide a good first approximation of flame temperature, specific heat ratio, impetus, and mean molecular weight of the combustion products. The program as developed at the Air Force Armament Laboratory was based on a code used by the National Aeronautics and Space Administration Lewis Research Center. The minor changes to the program are discussed, some results from advanced solid propellant formulations calculations are presented, and a form of users manual for thermochemical programs and for the program to generate specific heat polynomials from JANAF tabular data is presented.

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LIST OF ABBREVIATIONS AND SYMBOLS

C_p	Specific heat at constant pressure
C_v	Specific heat at constant volume
E	Internal energy
F_p	Propellant impetus
G	Gibbs free energy
H	Enthalpy
K	Gas conductivity
M	Molecular weight
P	Pressure
R	Gas constant
S	Entropy
T	Temperature
T_{FP}	Flame temperature at constant pressure
T_{FV}	Flame temperature at constant volume
V	Volume
X_i	Mole fraction
γ	Specific heat ratio
σ	Leonard-Jones force constant
Ω	Leonard-Jones force constant
μ	Gas viscosity

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SECTION I

INTRODUCTION

The field of gun propellant development, which had been relatively static for many years, has recently begun to attract increased attention. The availability of an accurate theoretical thermochemical propellant performance computer program is of central importance to informed research and development efforts in this field. As a formulation screening tool, a few dollars of machine time can save hundreds of dollars of laboratory small-batch-mix effort by eliminating unpromising candidate formulations and providing a good first approximation to the primary important propellant parameters. These would include flame temperature, specific heat ratio, impetus, and mean molecular weight of the combustion products. To most expediently obtain a computer program for computing the chemical equilibrium reaction products, the Air Force Armament Laboratory modified an existing free-energy minimization rocket propellant performance program. The program selected was the one used by the National Aeronautics and Space Administration Lewis Research Center. This code(1) has a background of almost ten years of successful application. In addition, it was readily available and the JANAF specific heat data could be easily applied to the thermodynamic data tape. The program, as modified for gun propellant applications, was checked against established experimental data and other analytic chemical equilibrium computing techniques, with excellent agreement. Additionally, an algorithm was added which computes combustion gas viscosity and thermal conductivity by a Leonard-Jones potential technique.

The following sections of this report discuss the minor changes made to the Lewis approach, give some results from advanced solid propellant formulation calculations, and provide a form of users manual for the thermochemical programs and for the program to generate specific heat polynomials form JANAF tabular data(2). Appendix I presents the Lewis program listing and Appendix II presents the polynomial fit program used at the Armament Laboratory.

SECTION II

FREE ENTHALPY EQUATIONS

This report will not discuss the mathematical techniques of chemical equilibrium computations. This task has effectively been accomplished in a recently issued monograph[3] which discusses in detail not only the Lewis technique but also several other commonly used approaches. This report will demonstrate only that, at chemical equilibrium, the Gibbs free energy, G, (or free enthalpy) will be a minimum.

From the First Law of Thermodynamics, in an irreversible process:

$$dE + pdv - Tds<0 \tag{1}$$

or at equilibrium

$$dE + pdv - Tds=0 \tag{2}$$

For a constant pressure and temperature, equation (2) becomes

$$d(E + pv - Ts) =0 \tag{3}$$

$$G_T = H_T - T_1S_1 \tag{4}$$

Equation (4) establishes the relation that the Gibbs free energy will be a minimum at equilibrium, and when coupled with the atomic species mass conservation equations, it provides a sufficient set for solution of the combu tion species concentration and flame temperature (if the combustion pressure is specified). Then, to set up a minimization algorthm only requires a value for the heat of formation of the reactant compounds and tabular or polynomial data for the specified heat, C_p, enthalpy, H_T, and entropy, S_T, of the possible combustion products. These thermodynamic data can be obtained from reference 2 for most combustion products of interest: as

$$H_T - H_{298} = \int_{298}^{T} C_p \, dT \tag{5}$$

and $$S_T - S_{298} = \int_{298}^{T} \frac{C_p}{T} \, dT \tag{6}$$

Selecting a polynomial form for C_p, the terms H_T and S_T can be conveniently fitted to similar polynomials by performing the indicated integrations

$$\frac{C_p}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \tag{7}$$

$$\frac{H_T}{RT} = a_1 + 1/2\ a_2T + 1/3\ a_3T^2 + 1/4\ a_4T^3 + 1/5\ a_5T^4 + a_6/T \tag{8}$$

$$\frac{S_T}{R} = a_1 LnT + a_2T + 1/2\ a_3T^2 + 1/3\ a_4T^3 + 1/4\ a_5T^4 + a_7 \tag{9}$$

For a more precise fit, the Lewis program utilizes two sets of coefficients for each species, one in the temperature range 0° to 1000°K and the other from 1000° to 6000°K. Limits of species existence can be placed on the propellant data to restrict the range of polynomial applicability.

The primary change made to the Lewis algorithm was to additionally develop an approximate isochoric temperature from the isobaric temperature provided by the program. This requires the assumption that approximately the same species would form either in an isochoric or isobaric process, providing a similar total heat release. If these assumptions are warranted, then:

$$Q_R = C_pT_{Fp} \tag{10}$$

$$Q_R = C_VT_{FV} \tag{11}$$

$$T_{FV} = C_p/C_VT_{Fp} = \gamma T_{Fp} \tag{12}$$

Once the isochoric flame temperature and mean molecular weight of the combustion products are known, the impetus is simply

$$F_p = \frac{R}{M}\ T_{FV} \tag{13}$$

where R = 2780 ft-lbs/lb-mole-°K

The program also computes the constitutive products mole fractions as a function of the pressure ratio (or, for a gun system, of the velocity) if quasi-isentropic conditions are assumed.

Equation (13) indicates the importance of developing advanced propellants with lower molecular weight combustion products, if the impetus

of a propellant is to be increased without a corresponding flame temperature increase. High propellant flame temperatui s are, of course, the prime limiting factor in developing an acceptable barrel life for automatic aircraft cannon having a high performance and a high rate of fire. Current single-base solid gun propellants display molecular weights in the order of 25. Table I illustrates the distinctive flame temperature advantage of lower molecular weights in obtaining cooler combustion conditions without sacrificing energy output.

TABLE I. FLAME TEMPERATURES AS A FUNCTION OF MOLECULAR WEIGHT AND IMPETUS

Molecular Weight, Atomic Mass Units	Flame Temperature, °K, at Impetus, Ft-lb/lb			
	325,000	350,000	375,000	400,000
25	2980	2150	3380	3500
22	2570	2770	2970	3170
20	2340	2620	2700	2880
19	2220	2390	2570	2740
18	2110	2270	2430	2590
17	1990	2140	2290	2450

The very favorable performance data indicated by the lower right-hand entries in Table I are responsible for the continued advanced solid gun propellant development efforts. The test cases described in the following sections have resulted from calculations of two of the formulations now under contract investigation and from a comparison of results of two theoretical computations with experimental measurements of inservice propellants. All computations are performed at a standard reference pressure of 5,000 psia.

The first requirement for free energy computations is a reliable list of heats of formations for the constituents to be considered. Table II provides this data for the ingredients in the formulations discussed in this report. Additional tables are available in references 4 and 5.

TABLE II. HEATS OF FORMATION

CONSTITUENT	EMPIRICAL FORMULA	HEATS OF FORMATION KILOCALORIES PER MOLE
Ammonium Nitrate	$H_4\ O_3\ N_2$	-88.1
CTPB	$C_7\ H_{11}\ O_{0.2}\ N_{0.02}$	-5.0
Dibutylphthalate	$C_{18}\ H_{14}\ O_4$	-200.0
Diphenylamine	$C_{12}\ H_{11}\ N_1$	+27.6
DMDTH	$C_6\ H_{14}\ O_6\ N_4$	-94.0
Ethyl Acrylate	$C_5\ H_8\ O_2$	-87.3
Ethyl Alcohol	$C_2\ H_6\ O_1$	-66.3
Ethyl Centralite	$C_{17}\ H_{20}\ O_1\ N_2$	-34.2
Ethylene Dihydrazine	$C_2H_{10}N_4$	+31.2
Glycol Dinitrate	$C_2\ H_4\ O_6\ N_2$	-58.7
Guanidine Nitrate	$C_1\ H_6\ O_3\ N_4$	-79.3
HMX	$C_4\ H_8\ O_8\ N_{812}$	+17.9
Nitrocellulose (12.6 percent N)	$C_{24}\ H_{30.2}\ O_{39.4}\ N_{9.8}$	-655.5
Nitrocellulose (12.7 percent N)	$C_{24}\ H_{30}\ O_{40}\ N_{10.0}$	-659.3
Nitrocellulose (13.15 percent N)	$C_{24}\ H_{29.5}\ O_{41.3}\ N_{10.6}$	-643.1
Nitrocellulose (13.75 percent N)	$C_{24}\ H_{29.3}\ O_{41.4}\ N_{10.7}$	-639.9
Nitroglycerine	$C_3\ H_5\ O_9\ N_3$	-85.3
Nitroguanidine	$C_1\ H_4\ O_2\ N_4$	-12.6
Polymethyl Vinyl Tetrazole	$C_4\ H_6\ N_4$	+52.4
RDX	$C_3\ H_6\ O_6\ N_6$	+14.9
Potassium Sulfate	$K_2\ S_1\ C_4$	-338.5
Triacetin	$C_9\ H_{14}\ O_6$	-307.0
Triazoethanol	$C_2\ H_5\ O_1\ N_3$	+22.5
Triaminoguanidine Nitrate	$C_1\ H_9\ O_3\ N_7$	-11.5
Water	$H_2\ O_1$	-68.4

SECTION III

COMPUTATION OF VISCOSITY AND CONDUCTIVITY

For gun propellant applications, it is often quite important to determine a theoretical value for the combustion gas conductivity and viscosity. These are particularly necessary if the convective gun barrel heating characteristics of the propellants are to be evaluated. To accomplish this task, the Leonard-Jones potential technique[6] was applied.

The viscosity for a single constitutive species is given by:

$$\mu_i = 2.6693 \times 10^{-5} \sqrt{MT} / \sigma^2 \Omega \tag{14}$$

where T is the temperature, M is the molecular weight, and σ and Ω are the Leonard-Jones force constants. The viscosity of the mixture is defined by

$$\mu_{MIX} = \sum_{i=1}^{n} \left(x_i \mu_i \right) \Bigg/ \left(\sum_{j=1}^{n} x_j \Phi_{ij} \right) \tag{15}$$

with n being the number of species considered and x_i being the mole fraction of the species. The value, Φ_{ij} is defined as

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j} \right)^{-1/2} \left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{1/2} \left(\frac{M_j}{M_i} \right)^{1/4} \right]^2 \tag{16}$$

The thermal conductivity of a species is given as:

$$K_i = 1.9891 \times 10^{-4} \frac{\sqrt{T/M}}{\sigma^2 \Omega} \tag{17}$$

The mixture value is given as

$$K_{MIX} = \sum_{i=1}^{n} \left(x_i k_i \right) \Bigg/ \left(\sum_{j=1}^{n} x_j \Phi_{ij} \right) \tag{18}$$

This approach is strictly valid for only dilute mixtures of non-polar molecules. Five species are considered, (one of which, H_2O, is polar), and all have a dense gas system. Thus, the results contain only order of magnitude validity, but are none the less of value, considering the state of the art in mathematical modeling of the transient heat convection process in gun bores. Table III gives the species considered which are typically 98 to 99 percent of the combustion gas constitutients.

TABLE III. LEONARD-JONES POTENTIAL PARAMETERS (FORCE CONSTANTS)			
Species	Molecular Weight, Atomic Mass Units	Viscosity, Grams/cm-sec	Conductivity, Cal/cm-sec-K
H_2	2.016	2.915	38.0
N_2	28.02	3.749	79.8
CO	28.01	3.706	88.
CO_2	44.01	3.897	213.
H_2O	18.0	2.824	230.9

Table IV consists of the Ω-$\frac{KT}{\epsilon}$ relations needed for the solution of Equations (14) and (17). The first column contains values for the relatively non-polar species such as H_2, N_2, CO, and CO_2, while the second column has a corrected value for the highly polar H_2O.

TABLE IV. REDUCED CROSS SECTION

KT/ε	NON-POLAR	POLAR		KT/ε	NON-POLAR	POLAR
1.0	1.5938	2.6199		7	0.8725	0.8946
1.2	1.4568	2.4257		8	0.8536	0.8422
1.4	1.3557	2.2713		9	0.8378	0.8043
1.6	1.2800	2.1413		10	0.8242	0.7760
1.8	1.2216	2.0263		11	0.8123	0.7544
2.0	1.1751	1.9217		12	0.8017	0.7376
2.2	1.1377	1.8258		13	0.7922	0.7243
2.4	1.1066	1.7373		14	0.7836	0.7134
2.6	1.0803	1.6559		15	0.7756	0.7045
2.8	1.0579	1.5812		16	0.7883	0.6971
3.0	1.0385	1.5126		32	0.6939	0.6462
3.2	1.0214	1.4499		64	0.6262	0.6033
3.4	1.0063	1.3926		128	0.5634	0.5528
3.6	0.9928	1.3401		256	0.5056	0.5006
3.8	0.9807	1.2922		512	0.4528	0.4505
4.0	0.9696	1.2485				
5.0	0.9265	1.0797				
6 0	0.8960	0.9694				

SECTION IV

INPUT FOR GUN PROPELLANT PROGRAM

The input data for the gun propellant program (Appendix I) can be divided into four general groups having code names as follows:

1) Thermodynamic data for the reaction products (THERMØ data).
2) Data pertaining to the reactants or propellants (REACTANTS data).
3) Special options related to chemical species present in the combusted gas (ØMIT/INSERT data).
4) Namelist data including the type of problem, pressure ratio and area ratio schedules, various options, etc. (NAMELISTS data).

The required order of the data cards is:

1) One card with the code word THERMØ punched in columns 1 to 6.
2) THERMØ data.
3) REACTANTS card. Number of reactants right adjusted in columns 1 to 3 and number of cases right adjusted in columns 4 to 6.
4) ØMIT and/or INSERT data.
5) One card containing up to 80 columns of alphanumeric identification data.
6) NAMELISTS data.

For any particular problem there may be multiple REACTANTS cards. Each set of REACTANTS cards may be followed by multiple NAMELISTS input cards. Each type of input data is discussed in detail in the following sections.

1. THERMØ DATA

The thermodynamic data for the reaction products may be read either from cards or from magnetic tape. When tape input is used, both the THERMØ code card and all THERMØ data cards must be omitted. It is anticipated that most users will prefer the magnetic tape since this reduces the number of cards which must be handled. The card format for the THERMØ data is described in Section V. Use of the tape input requires no action on the part of the user, once the required data is established on the tape.

2. REACTANTS DATA

REACTANTS data is required for all problems. Following the code card there should follow one card for each reactant species being considered, with a maximum of 15 allowed. Each reactant card, after the code card, contains the following information:

a. The chemical formula for the species.

b. Either the number of moles of the reactant or the relative weight. The relative weight is the weight of each fuel or oxidizer expressed as a fraction of the total fuel or oxidizer.

c. The enthalpy of the species expressed in calories per mole. (This is not required for an assigned temperature problem. See Section IV.4 for description of assigned temperature problem.)

d. The state of the reactant (gas, liquid, or solid).

e. The temperature associated with the enthalpy.

f. Designation of each reactant species as either a fuel or an oxidizer. (The program then combines all fuels into an effective fuel and all oxidizers into an effective oxidizer.)

g. The reactant species density. (This information is optional and may be omitted. If densities are input for all reactants, the program calculates a density for the overall system.)

h. Multiple cases with identical reactants are identified by the reactants code card and the preceding data need not be repeated.

The reactant information is arranged on a card. Standard chemical alphabetic symbols are required for the chemical elements (i.e., H for hydrogen, HE for helium, LI for lithium, BE for beryllium, etc.). Each reactant may be composed of no more than five distinct chemical elements. Each chemical element is allowed two columns (columns 1 and 2, 10 and 11, 19 and 20, 28 and 29, and 37 and 38) for its symbol. For those elements whose symbol consists of a single letter, the symbol must be placed in the left-most (left adjusted) of the two columns. The formula number (the number of atoms of each element in a reactant) is to appear in the columns immediately following the chemical symbol (i.e., columns 3 to 9, 12 to 18, 21 to 27, 30 to 36, and 39 to 45). The formula number may appear anywhere within the seven column field, and a decimal point must be used for each number. Note that the exponent numeric form, or E format, may not be used here. Also note that for a given reactant an individual element may appear only once (empirical formula). Thus, a compound such as furfuryl alcohol, whose formula might be written as C4H3O·CH2OH to represent its structure, must be treated as though it were C5H6O2 or O2H6C5, etc. The order of the elements is immaterial for this program.

The relative weight of each reactant should be placed in columns 46 to 52. The number may appear anywhere in these columns, a decimal point must be used, and the exponent numeric form may not be used. If the number of moles of each species is input in these columns the same restrictions apply, but an additional bit of information, an M in column 53, must

appear on the card. Column 53 is left blank for relative weights. Note that the relative weight and molar designations may not be mixed for any single problem.

The reactant enthalpy is placed in columns 54 to 62, and the units must be calories per mole. The number may appear anywhere in these columns, a decimal point must be used, and the exponent numeric form may not be used. A sign is required only if the enthalpy is negative. Obviously, this enthalpy must be consistent with the enthalpy base used for the THERMØ data. For the JANAF data, the enthalpy base is as follows: For each element, the phase, condensed or liquid, which is most stable at one atmosphere pressure is designated as a reference, or base, state. The heat of formation of this state at 298.15°K is arbitrarily specified as zero. Then all thermodynamic properties for other phases of the element, as well as for any compound containing the element, are referenced to the base state.

The initial state for each reactant is indicated by an S for solid, an L for liquid, or a G for gas in column 63. The initial reactant temperature, in degrees Kelvin, goes in columns 64 to 71. Both the initial state and temperature are used only to label the output printout and if they are omitted or input incorrectly, the calculations are not affected.

For all problem types (see Section IV.4) except a detonation problem, columns 73 to 70 are reserved for the reactant density in grams per cubic centimeter. The inputting of this data is optional, but if it is given, a decimal point must be used. For a detonation problem, columns 73 to 80 are used for the reactant specific heat at constant pressures. This data is required for each reactant for a detonation problem

3. ØMIT/INSERT DATA

The purpose of the ØMIT/INSERT option is as follows. The program considers as possible products all species in the THERMØ data which are consistent with the chemical system which was input on the REACTANTS cards. Occasionally, it may be desired to eliminate one or more species from consideration as possible products. This may be accomplished by placing the species chemical formula on an ØMIT card. Both gaseous and condensed species may be omitted.

Only the names of condensed species may appear on an INSERT card. The INSERT option has been included for two reasons. The less important of the two is that if it is known beforehand that one or more particular condensed species will be among the final equilibrium composition for the first assigned point (i.e., the combustion chamber for a rocket problem), then a small amount of computer time can be saved by using an INSERT card. The more important reason for the INSERT option is that, in rare instances, it is impossible to obtain convergence without the use of an

INSERT card. This occurs when, by considering gases only, the temperature becomes extremely low. When this happens, the program outputs the following message: "LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE BEEN INCLUDED ON AN INSERT CARD" and no solution will be obtained. The user should resubmit the problem with one or more appropriate condensed species listed on an INSERT card.

The use of ØMIT and INSERT cards is completely optional; however when used, each card must contain either the code word ØMIT in columns 1 to 4 or INSERT in columns 1 to 6 and the chemical formulas of from one to four product species. The names of the species must be left-adjusted and begin in columns 16, 31, 46, or 61. In addition, the species name must be punched on the card exactly as it appears in the THERMØ data. This means that the order of the chemical elements within the species name, the formula numbers, and the state of the species must all be identical. For example, gaseous ammonia would commonly appear as NH_3. Because of the alphabetizing scheme used for thermodynamic data, this species is written as H3N1(G).

4. NAMELISTS DATA

The word NAMELIST is a FØRTRAN IV statement and provides a convenient way of inputting data. One of the major advantages of the NAMELIST input method is that the data can be placed in any order and need not be placed within pre-specified card columns as is the case for the REACTANTS data. A secondary advantage is that the variable name appears with its numerical value on a card, thus making it easy to tell the purpose of each piece of data without having to refer to a program manual or to the program listing. Even though inputting data by means of NAMELIST is convenient, the following rules must be observed.

All data input by means of a NAMELIST statement must be associated with a NAMELIST name, and for this program there are only two: INPT2 and RKTINP. The first column of all NAMELIST data cards may not be used and must be blank. The second column of the first card only must contain a $ character. The applicable NAMELIST name must be placed on the first card only. The name must begin in column 3, and must be followed by at least one blank column.

Each NAMELIST name is assigned a group of FØRTRAN variables. (The variables belonging to INPT2 and RKTINP are listed in Tables V and VI, respectively.) These variables are assigned to a NAMELIST name within the program, and numeric data can only be input in conjunction with a NAMELIST name.

Although, in general, there are seven forms that input data may take, only three are of interest for this report. These are integer constants,

real number constants, and logical constants. These are defined as follows:

a. An integer consists of one to eleven digits written without a decimal point.

b. A real number constant may be written in two ways. The first form is from one to nine digits, including a decimal point, followed by an exponent. The exponent is written as the letter E followed by a sign and a one or two digit integer. For example 12345. could be written as 1.2345E04 or .12345+5, etc. The second form is one to nine digits, including a decimal point, but not followed by an exponent.

c. A logical constant may be either true or false. There are two forms in which the constant may be written. These are either .TRUE. or T .FALSE. or F. The periods before and after the long forms are mandatory.

Logical constants may be associated only with logical variables. Integer constants may be associated with real variables and vice versa, and the proper conversion is made automatically by the computer. Note that when inputting data without a NAMELIST statement this conversion may cause difficulties and should only be used with great care.

On a NAMELIST card, each piece of data must be written in conjunction with its variable name (e.g., P = 100, or INDEX = 3, or PSIA = .TRUE., etc.). The equal sign is mandatory, and the data items must be separated by commas. If more than one card is required, the last item on each card, except for the last card, must be a constant followed by a comma. A variable name may not be the last item on the card. The end of a group of data is signaled by a $ character. This may be on the same card as that containing the NAMELIST name if only one card is used or may be on any succeeding card, but it may not be the first character on a succeeding card. Note that it is not necessary to completely fill a card with data before beginning a subsequent card. In fact, the user may want to put each piece of data on separate cards. This facilitates subsequent data changes. One final note, it is not necessary to input data for every variable contained in a NAMELIST; however, each variable has been assigned a value within the program, and this value is used unless superseded by input data. The assigned values for all NAMELIST variables in this program are included in Tables V and VI.

To illustrate the preceding instructions, the following paragraphs discuss the specific NAMELIST data required by this program, what each data bit does, and then some specific examples.

The INPT2 NAMELIST data must be used for all problems. The variables in the INPT2 NAMELIST are listed and defined in Table V along with the type and assigned value of each variable. The type of problem (one of either TP, HP, RKT, or DETN), at least one pressure (P), and the relative amounts of fuel and oxidizer (i.e., one of either EQRAT, OF, FPCT, or FA) are required for each problem. The other variables are either completely optional or may be required only if a particular problem type is requested.

The variable JANF is a flag to indicate which thermodynamic data polynomial should be used. JANF=0 designates a polynomial of the form $C_p=A_1+A_2T+A_3T^2+A_4T^3+A_5T^4$. This is the form used by the Lewis Research Center and is also the form the Armament Laboratory uses after converting the JANAF data.

The Lewis program is quite flexible in the type of problems it will consider or the thermodynamic variables which may be fixed. For gun propellant problems, it is most advantageous to assign the enthalpy and pressure which, in system nomenclature, constitutes an RKT problem.

a. RKT Problem

If RKT = .TRUE. or T, then a rocket problem is solved. A rocket problem is one for which the combustion takes place at an assigned enthalpy (REACTANTS cards) and assigned pressure (single value in the P variable), followed by an isentropic expansion. The combustion temperature, the thermodynamic properties and rocket performance are calculated for the chamber, the throat, and assigned exit points. The exit points desired are specified in the RKTINP namelist. If a temperature is assigned (T variable), then combustion will be assumed to occur at that temperature and not at the assigned enthalpy. The RKT problem type combines the H,S and T,S problems of the earlier program version. Note that, when this option is selected, the second set of NAMELIST data, RKTINP, is then required. The combustion gas conductivity and viscosity are computed for this option only.

b. DETN Problem

If DETN = .TRUE. or T, then the program solves a Chapman-Jouget detonation problem. The thermodynamic properties and composition downstream of the detonation wave are calculated for an assigned pressure and temperature upstream of the wave. This detonation calculation is primarily oriented for gas phase detonations. It is of limited utility for computation of detonations in solids, as the specific heat polynomial of the reactants must be on the data tape, which will not, in general, be the case for a typical solid explosive constituent ingredient.

c. P, PSIA, and MMHG Variables

The value P may be either the combustion pressure of a rocket engine (RKT problem) or a pressure at which composition and thermodynamic properties (TP or HP problem) are desired. Up to 26 values may be input, but only one is permitted for an RKT problem. The program assumes that the units of the pressures are in atmospheres unless either PSIA or MMHG are set true. If PSIA = .TRUE. or T then the pressure units are assumed to be in psia units. If MMHG = .TRUE. or T then the pressure units are assumed to be in millimeters of mercury. PSIA and MMHG may not both be set true in the same problem.

d. T Variable

Values for the T variable should be input only if TP is set true or if an assigned chamber temperature is desired for RKT problem. The temperature units must be degrees Kelvin.

e. EQRAT, ØF, FPCT, and FA Variables

The relative amounts of total fuel and total oxidizer may be expressed in one (and only one for each problem) of four ways. The mixture ratio (ØF) and percent fuel (FPCT) are self evident. The fuel-to-air weight ratio (FA) and equivalence ratio (EQRAT) are new to this version of the program and are not of use for gun propellant calculations.

f. IDEBUG Variable

If IDEBUG = .TRUE. or T then a printout of the intermediate calculation details is obtained. This is intended primarily as a debugging aid in the event there are problems. The output is extensive and is explained on page 34 of Reference 1.

g. IØNS Variable

If IØNS = .TRUE. or T then the program will consider ionized species. The earlier Lewis program version could not handle ionic species although provision was made in one of the subroutines for future consideration of ions. This capability is included in the newer program and thermodynamic data for ionized species are available as well as a sample problem which uses IØNS = T.

h. EQL, FRØZ, PCP, SUBAR, and SUPAR Variables

The five RKTINP variables (EQL, FRØZ, PCP, SUBAR, and SUPAR) in the RKTINP namelist are listed in Table VI. Of these, only PCP is required. The RKTINP namelist is required only if RKT is set true in the INPT2 namelist.

(1) PCP Variable

The value PCP is the ratio of the chamber pressure to the exit pressure. This is one of the independent variables (along with the entropy) for the nozzle portion of a rocket problem, and as such, at least one value must be input. As many as 22 values may be input; however, unlike the older program, values for the chamber and throat should not be input. Pressure ratios for the subsonic portion of the nozzle may be used. Values must be ordered so that the magnitudes increase monotonically.

(2) SUBAR and SUPAR Variables

Gun propellant performance at specific area ratios corresponding to a given gas velocity, either subsonic or supersonic, may be requested. Subsonic ratios are read as SUBAR and supersonic as SUPAR. When assigned area ratios are requested, the range of PCP values should be large enough to include the assigned area ratios. If the range is not large enough, extrapolation may be performed. SUBAR values should be ordered such that the values decrease and the SUPAR data should increase. Thirteen of each variable are permitted. Note that the use of this program feature is completely optional.

(3) EQL and FRØZ Variables

The program will calculate performance for both equilibrium and frozen expansions unless instructed otherwise. If EQL = .FALSE. or F then the equilibrium expansion is omitted and only frozen performance is calculated. If FRØZ = .FALSE. or F then the frozen expansion is omitted and only equilibrium performance is calculated.

TABLE V. VARIABLES IN INPT2 NAMELIST

Variable Name	Variable Type	Value (Unless Set Differently)	Definitions
JANF	Integer	1.	Thermodynamic data polynomial indicater
P	Real	0.	Assigned pressures
T	Real	0.	Assigned temperatures
EQRAT	Real	0.	Equivalence ratio
ØF	Real	0.	Oxidant-to-fuel weight ratio
FPCT	Real	0.	Percent fuel by weight
FA	Real	0.	Fuel-to-air weight ratio
TP	Logical	False	Assigned temperature and pressure problem
HP	Logical	False	Assigned enthalpy and pressure problem
RKT	Logical	False	Rocket problem
DETN	Logical	False	Detonation problem
PSIA	Logical	False	Assigned pressure to be in psia units
MMHG	Logical	False	Assigned pressures in millimeter of mercury units
IØNS	Logical	False	Consider ionic species
IDEBUG	Logical	False	Print intermediate output

TABLE VI. VARIABLES IN RKTINP NAMELIST

Variable Name	Variable Type	Value Unless Set Differently	Definition
EQL	Logical	True	Gun propellant performance assuming equilibrium composition to be calculated
FRØZ	Logical	False	Gun propellant performance assuming frozen composition to be calculated
PCP	Real	0.	Ratio of chamber pressure to exit pressure
SUBAR	Real	0.	Subsonic area ratios
SUPAR	Real	0.	Supersonic area ratios

Table VII contains the input data for several propellant performance cases, and the output is listed on Tables VIII through XI. These cases are respectively M-10 (Case 100), M-9 (Case 101), an HMX-rubber propellant system (Case 102), and an RDX-triamino-guanidine nitrate formulation (Case 106). A comparison of these data with experimental or independent theoretical solutions gives the following results.

	Tv	Fp	γ	Mw
Case 100				
Lewis	3312	366,548	1.22	25.1
Experimental	3034	346,180	1.23	24.2
Case 101				
Lewis	3853	394,180	1.17	27.2
Experimental	3840	396,840	1.20	26.5
Case 102				
Lewis	2566	377,584	1.28	18.9
Other Theoretical	2545	373,000	(--)	18.9
Case 106				
Lewis	2637	390,870	1.29	18.8
Other Theoretical	2647	391,000	(--)	18.8

The input data (Table VII) are discussed in the program writeup except that no ØMIT or INSERT cards are used.

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TABLE VII. INPUT DATA FOR SAMPLE GUN PROPELLANT PROBLEMS

```
  3  1
C 24.0    H 29.5    O 41.3    N 10.6                  1.0    -643100.   298.    F
C 12.0    H 11.0    N 1.0                             .33      27600.   298.    O
C 2.0     H 14.0    O 6.0     N 4.0                   .67     -66300.   298.    O
 CASE 100      PROPELLANT IS M-10
 $INPT2    JANF=0,P(1)=5000.,RKT=.TRUE.,FPCT=98.,PSIA=.TRUE.$
 $RKTINP   PCP(1)=1.2,1.4,1.6,2.0,3.0,4.0,5.0,10.0,68.0,FROZ=.FALSE.$
  4  1
C 24.0    H 29.5    O 41.3    N 10.6                  1.0    -643100.   298.    F
C 3.0     H 5.0     O 9.0     N 3.0                   .96     -85300.   298.    O
C 12.0    H 11.0    N 1.0     N 4.0                   .02      27600.   298.    O
C 3.0     H 14.0    O 6.0                             .02     -66300.   298.    O
 CASE 101      PROPELLANT IS M-9
 $INPT2    JANF=0,P(1)=5000.,RKT=.TRUE.,FPCT=58.,PSIA=.TRUE.$
 $RKTINP   PCP(1)=1.2,1.4,1.6,2.0,3.0,4.0,5.0,10.0,68.0,FROZ=.FALSE.$
  2  1
C 4.0     H 8.0     O 8.0     N 8.0                   1.0      17900.   298.    O
C 7.0     H 11.0    O .2      N .02                   1.0      -5000.   298.    F
 CASE 102      PROPELLANT IS HMX RUBBER
 $INPT2    JANF=0,P(1)=5000.,RKT=.TRUE.,FPCT=15.,PSIA=.TRUE.$
 $RKTINP   PCP(1)=1.2,1.4,1.6,2.0,3.0,4.0,5.0,10.0,68.0,FROZ=.FALSE.$
  3  1
C 4.0     H 8.0     O 8.0     N 8.0                   1.0      17900.   298.    O
C 7.0     H 11.0    O .2      N .02                   .88      -5000.   298.    F
TI1.0                                                 .12          0.   298.    F
 CASE 103      PROPELLANT IS HMX-RUBBER WITH TITANIUM ADDED
 $INPT2    JANF=0,P(1)=5000.,RKT=.TRUE.,FPCT=17.,PSIA=.TRUE.$
 $RKTINP   PCP(1)=1.2,1.4,1.6,2.0,3.0,4.0,5.0,10.0,68.0,FROZ=.FALSE.$
  4  1
C 2.0     H 5.0     O 1.0     N 3.0                   .83      22500.   298.    F
C 4.0     H 6.0     N 4.0                             .17      52400.   298.    F
C 3.0     H 6.0     O 6.0     N 6.0                   .60      14900.   298.    O
C 1.0     H 9.0     O 3.0     N 7.0                   .40     -11500.   298.    O
 CASE 106      PROPELLANT IS RDX-TAG NITRATE
 $INPT2    JANF=0,P(1)=5000.,RKT=.TRUE.,FPCT=16.,PSIA=.TRUE.$
 $RKTINP   PCP(1)=1.2,1.4,1.6,2.0,3.0,4.0,5.0,10.0,68.0,FROZ=.FALSE.$
```

TABLE VIII. OUTPUT FOR CASE 100, M-10 PROPELLANT

THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 5000.0 PSIA

CASE 100 PROPELLANT IS M-10

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C 24.00000	H 29.50000	O 41.30000	N 10.60000	1.00000	-643100.000		298.00	-0.0000
OXIDANT	C 12.00000	H 11.00000	N 1.00000		.33000	27600.000		298.00	-0.0000
OXIDANT	C 2.00000	H 14.00000	O 6.00000	N 4.00000	.67000	-66300.000		298.00	-0.0000

O/F= .0204 PERCENT FUEL= 98.0000 EQUIVALENCE RATIO= 1.5547 DENSITY= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.000	1.788	1.200	1.400	1.600	2.000	3.000	4.000	5.000	10.000	60.000
P, ATM	340.2	190.3	283.5	243.0	212.6	170.1	113.4	85.06	68.05	34.02	5.003
T, CP, DEG K	2713	2441	2625	2553	2491	2391	2217	2101	2015	1766	1227
H, CAL/G	-562.7	-681.0	-601.2	-632.7	-659.3	-702.4	-776.2	-825.3	-861.6	-965.8	-1189.2
S, CAL/(G)(K)	2.2442	2.2442	2.2442	2.2442	2.2442	2.2442	2.2442	2.2442	2.2442	2.2442	2.2442
M, MOL WT	25.125	25.137	25.130	25.133	25.135	25.138	25.141	25.143	25.143	25.144	25.148
(DLV/DLP)T	-1.00052	-1.00022	-1.00040	-1.00032	-1.00026	-1.00019	-1.00010	-1.00007	-1.00005	-1.00003	-1.00030
(DLV/DLT)P	1.0096	1.0040	1.0074	1.0058	1.0047	1.0033	1.0017	1.0010	1.0007	1.0003	1.0037
CP, CAL/(G)(K)	.4447	.4313	.4398	.4362	.4334	.4294	.4239	.4209	.4191	.4152	.4239
GAMMA (S)	1.2206	1.2263	1.2226	1.2241	1.2253	1.2272	1.2300	1.2316	1.2328	1.2352	1.2307
SON VEL,M/SEC	1046.8	995.0	1030.5	1016.7	1004.8	985.1	949.7	925.1	906.2	849.4	786.6
MACH NUMBER	0.000	1.000	.551	.753	.895	1.098	1.408	1.603	1.745	2.160	3.240
VEL, FT/SEC	0.0	3264.4	1861.8	2511.7	2950.7	3547.5	4385.6	4863.7	5188.8	6819.9	7512.1
VISC, G/CM-SEC	.000795	.000738	.000777	.000762	.000749	.000727	.000690	.000665	.000646	.000591	.000468
C, CAL/G-SEC-K	.000300	.000281	.000294	.000289	.000285	.000278	.000266	.000256	.000251	.000234	.000281
T, CV, DEG K	3312										
IMPETUS	366548.										
CSTAR, FT/SEC		4760	4760	4760	4760	4760	4760	4760	4760	4760	4760
CF		.686	.391	.528	.620	.745	.921	1.022	1.090	1.265	1.578
AE/AT		1.000	1.266	1.065	1.011	1.008	1.134	1.292	1.452	2.194	8.385
IVAC,LB-SEC/LB		184.2	213.9	190.5	185.1	184.8	192.3	199.0	204.2	219.6	251.5
I, LB-SEC/LB		101.5	57.9	78.1	91.7	110.3	136.3	151.2	161.3	187.1	233.5

TABLE VIII. Concluded

MOLE FRACTIONS

CH4	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00007
CO	.40188	.39739	.40060	.39943	.39834	.39637	.39279	.38896	.38611	.37568	.33827
CO2	.13746	.14230	.13888	.14019	.14130	.14335	[illegible]	.15091	.15378	.16431	.20966
H	.00104	.00046	.00082	.00066	.00054	.00039	.00020	.00012	.00008	.00002	.00000
HCN	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00000	.00000	.00000	.00000
HCO	.00016	.00068	.00013	.00011	.00009	.00007	.00004	.00002	.00002	.00001	.00000
H2	.10392	.10883	.10535	.10664	.10781	.10990	.11415	.11755	.12044	.13101	.17615
H2O	.23507	.23088	.23392	.23283	.23180	.22989	.22585	.22253	.21968	.20916	.16394
NH3	.00003	.00003	.00003	.00003	.00003	.00003	.00002	.00002	.00002	.00002	.00002
NO	.00005	.00001	.00004	.00002	.00002	.00001	.00000	.00000	.00000	.00000	0.00000
N2	.11974	.11983	.11978	.11980	.11982	.11984	.11986	.11987	.11987	.11987	.11989
OH	.00061	.00019	.00043	.00032	.00024	.00015	.00006	.00003	.00001	.00000	0.00000

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	C(S)	CH	CH2	CH3	CN	CH2	C2	C2H	C2H2
C2H4	C2N	C2N2	C2O	C3	HO2	H2O(L)	H2O(S)	N	NH
NH2	NO2	N2C	N2H4	N2O	N2O4	O	O2		

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

VISCOSITY AND CONDUCTIVITY VALUES BASED ON 99.8 PERCENT OF GAS MIXTURE

TABLE IX. OUTPUT FOR CASE 101, M-9 PROPELLANT

THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 5800.0 PSIA

CASE 101 PROPELLANT IS M-9

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C 24.00000	H 29.50000	O 41.30000	N 10.60000	1.00000	-643100.000		298.00	-0.0000
OXIDANT	C 3.00000	H 5.00000	O 9.00000	N 3.00000	.96000	-85300.000		298.00	-0.0000
OXIDANT	C 12.00000	H 11.00000	N 1.00000	N 4.00000	.02000	27660.000		298.00	-0.0000
OXIDANT	C 3.00000	H 14.00000	O 6.00000		.02000	-66300.000		298.00	-0.0000

O/F= .7241 PERCENT FUEL= 58.0000 EQUIVALENCE RATIO= 1.3101 DENSITY= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.000	1.759	1.200	1.400	1.600	2.000	3.000	4.000	5.000	10.000	68.000
P, ATM	340.2	193.4	283.5	243.0	212.6	170.1	113.4	85.06	68.05	34.02	5.003
T, CP, DEG K	3298	3049	3217	3149	3091	2992	2815	2690	2594	2310	1648
H, CAL/G	-485.1	-615.8	-528.5	-564.3	-594.6	-644.0	-729.4	-786.8	-829.5	-952.5	-1224.6
S, CAL/(G)(K)	2.2389	2.2389	2.2389	2.2389	2.2389	2.2389	2.2389	2.2389	2.2389	2.2389	2.2389
M, MOL WT	27.185	27.319	27.234	27.271	27.300	27.342	27.398	27.426	27.441	27.466	27.477
(DLV/DLP)T	-1.00614	-1.00326	-1.00508	-1.00429	-1.00366	-1.00276	-1.00157	-1.00101	-1.00070	-1.00021	-1.00001
(DLV/DLT)P	1.1238	1.0700	1.1051	1.0904	1.0786	1.0611	1.0364	1.0242	1.0173	1.0055	1.0001
CP, CAL/(G)(K)	.6142	.5393	.5888	.5680	.5509	.5245	.4849	.4636	.4507	.4253	.4038
GAMMA (S)	1.1685	1.1784	1.1713	1.1740	1.1765	1.1818	1.1892	1.1947	1.1985	1.2074	1.2163
SON VEL,M/SEC	1085.6	1045.7	1072.6	1061.7	1052.3	1036.6	1007.3	987.0	970.6	918.8	779.5
MACH NUMBER	0.000	1.000	.562	.767	.910	1.112	1.419	1.610	1.749	2.152	3.191
VEL, FT/SEC	0.0	3430.7	1976.6	2670.2	3140.5	3782.7	4691.1	5213.1	5569.8	6488.1	8161.4
VISC, G/CM-SEC	.000906	.000866	.000895	.000884	.000874	.000856	.000824	.000799	.000779	.000719	.000572
C, CAL/G-SEC-K	.000291	.000278	.000287	.000283	.000280	.000274	.000265	.000257	.000252	.000235	.000195
T, CV, DEG K	3353										
IMPETUS	394 [illegible]										
CSTAR, FT/SEC		5121	5121	5121	5121	5121	5121	5121	5121	5121	5121
CF		.670	.386	.521	.613	.739	.916	1.018	1.088	1.267	1.594
AE/AT		1.000	1.253	1.058	1.006	1.011	1.148	1.315	1.483	2.265	8.734
IVAC,LB-SEC/LB		197.1	227.7	203.3	197.9	198.0	206.7	214.4	220.3	237.7	274.1
I, LB-SEC/LB		106.6	61.4	83.0	97.6	117.6	145.8	162.0	173.1	201.7	253.7

TABLE IX. Concluded

MOLE FRACTIONS

CO	.27808	.27371	.27656	.27535	.27438	.27285	.27035	.26867	.26735	.26277	.24173
CO2	.21989	.22997	.22194	.22344	.22496	.22727	.23084	.23583	.23463	.23969	[illegible]
H	.00427	.00288	.00380	.00342	.00318	.00260	.00180	.00134	.00104	.00042	.00001
HCO	.00016	.00009	.00013	.00012	.00010	.00006	.00005	.00004	.00003	.00001	.00000
HO2	.00001	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	0.00000	0.00000
H2	.04746	.04847	.04769	.04795	.04824	.04883	.05026	.05156	.05272	.05721	.07039
H2O	.28839	.29217	.28987	.29093	.29170	.29268	.29347	.29338	.29279	.28943	.26877
NH2	.00001	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	0.00000
NH3	.00001	.00001	.00001	.00001	.00001	.00000	.00000	.00000	.00000	.00000	.00000
NO	.00243	.00116	.00195	.00160	.00133	.00095	.00048	.00027	.00017	.00003	.00000
N2	.14733	.14870	.14784	.14822	.14851	.14693	.14948	.14973	.14987	.15088	.15815
O	.00058	.00022	.00044	.00034	.00026	.00017	.00007	.00003	.00002	.00000	0.00000
OH	.01079	.00607	.00911	.00780	.00676	.00521	.00303	.00195	.00134	.00034	.00000
O2	.00140	.00054	.00106	.00092	.00064	.00041	.00016	.00008	.00004	.00000	0.00000

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	C(S)	CH	CH2	CH3	CH4	CN	CN2	C2	C2H
C2H2	C2H4	C2N	C2N2	C2O	C3	HCN	H2O(L)	H2O(S)	N
NH	NO2	N2C	N2[illegible]4	N2O	N2O4				

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

VISCOSITY AND CONDUCTIVITY VALUES BASED ON 98.0 PERCENT OF GAS MIXTURE

TABLE X. OUTPUT FOR CASE 102, HMX-RUBBER

THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 5000.0 PSIA

CASE 102 PROPELLANT IS HMX-RUBBER

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT	C 4.00000	H 8.00000	O 8.00000	N 8.00000	1.00000	17900.000		298.00	-0.0000
FUEL	C 7.00000	H 11.00000	O .20000	N .02000	1.00000	-5800.000		298.00	-0.0000

O/F= 5.6667 PERCENT FUEL= 15.0000 EQUIVALENCE RATIO= 2.7550 DENSITY= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.000	1.819	1.200	1.400	1.600	2.000	3.000	4.000	5.000	10.000	68.000
P, ATM	340.2	187.0	283.5	243.0	212.6	170.1	113.4	85.06	68.05	34.02	5.003
T, CP, DEG K	1995	1758	1918	1856	1905	1724	1592	1510	1453	1310	1070
H, CAL/G	43.8	-73.8	6.3	-24.2	-49.8	-91.0	-160.9	-207.0	-241.0	-337.8	-557.9
S, CAL/(G)(K)	2.4686	2.4686	2.4686	2.4686	2.4686	2.4686	2.4686	2.4686	2.4686	2.4686	2.4686
M, MOL WT	18.902	19.006	18.925	18.950	18.976	19.030	19.163	19.264	19.392	19.796	21.091
(DLV/DLP)T	-1.01474	-1.02159	-1.01644	-1.01815	-1.01982	-1.02299	-1.02975	-1.03507	-1.03932	-1.05817	-1.07938
(DLV/DLT)P	1.0946	1.1603	1.1127	1.1309	1.1489	1.1839	1.2631	1.3303	1.3876	1.7068	2.2465
CP, CAL/(G)(K)	.5308	.5951	.5452	.5607	.5769	.6103	.6929	.7693	.8383	1.3712	2.3570
GAMMA (S)	1.2863	1.2791	1.2854	1.2837	1.2817	1.2769	1.2642	1.2531	1.2438	[illegible]	1.1394
SON VEL,M/SEC	1062.5	991.7	1040.8	1022.5	1006.7	980.7	934.5	903.3	880.2	809.4	693.4
MACH NUMBER	0.000	1.000	.538	.738	.879	1.083	1.400	1.604	1.754	2.208	3.2[illegible]
VEL, FT/SEC	0.0	3253.6	1837.3	2474.8	2903.8	3484.2	4293.7	4752.8	5064.5	5862.5	7361.[illegible]
VISC, G/CM-SEC	.000604	.000555	.000588	.000576	.000565	.000548	.000521	.000504	.000493	.000469	.000416
C, CAL/G-SEC-K	.000391	.000357	.000380	.000371	.000364	.000351	.000331	.000317	.000307	.000285	.000249
T, CV, DEG K	2566										
IMPETUS	377584.										
CSTAR, FT/SEC		4627	4627	4627	4627	4627	4627	4627	4627	4627	4627
CF		.703	.397	.535	.628	.753	.928	1.027	1.095	1.267	1.591
AE/AT		1.000	1.250	1.072	1.014	1.008	1.123	1.279	1.431	2.184	9.087
IVAC,LB-SEC/LB		180.2	210.6	187.0	181.4	180.6	187.3	193.6	198.6	213.6	248.0
I, LB-SEC/LB		101.1	57.1	76.9	90.3	108.3	133.5	147.7	157.4	182.2	228.8

TABLE X. Concluded

MOLE FRACTIONS

C(S)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	.00998	.87542
CH3	.00003	.00001	.00002	.00002	.00001	.00001	.00000	.00000	.00000	.00000	.00000
CH4	.00418	.00735	.00494	.00571	.00649	.00805	.01175	.01508	.01803	.02372	.02120
CO	.40682	.40490	.40640	.40595	.40546	.40443	.40181	.39928	.39691	.37715	.27309
CO2	.00566	.00741	.00608	.00650	.00693	.00780	.00992	.01194	.01383	.02277	.06092
C2H2	.00002	.00001	.00002	.00001	.00001	.00001	.00000	.00000	.00000	.00000	0.00000
C2H4	.00002	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00000
H	.00005	.00001	.00003	.00002	.00001	.00001	.00000	.00000	.00000	.00000	0.00000
HCN	.00136	.00074	.00114	.00098	.00085	.00067	.00043	.00030	.00023	.00009	.00381
HCO	.00007	.00002	.00005	.00004	.00003	.00002	.00001	.00000	.00000	.00000	.00000
H2	.34336	.33876	.34237	.34127	.34009	.33764	.33162	.32618	.32141	.30765	.28640
H2O	.02153	.02240	.02165	.02185	.02210	.02266	.02413	.02545	.02656	.03329	.05793
NH3	.00065	.00056	.00062	.00060	.00057	.00054	.00049	.00045	.00042	.00033	.00015
N2	.21627	.21782	.21806	.21704	.21742	.21814	.21982	.22129	.22259	.22510	.22480

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CN	CN2	C2	C2H	C2N	C2N2	C2O
C3	HO2	H2O(L)	H2O(S)	N	NH	NH2	NO	NO2	N2O
N2H4	N2O	N2O4	O	OH	O2				

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

VISCOSITY AND CONDUCTIVITY VALUES BASED ON 99.4 PERCENT OF GAS MIXTURE

TABLE XI. OUTPUT FOR CASE 106, RDX-TRIAMINO GUANIDINE NITRATE

THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 5000.0 PSIA

CASE 106 PROPELLANT IS RDX-TAG NITRATE

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C	2.00000	H	5.00000	O	1.00000	N	3.00000	.83000	22500.000		298.00	-0.0000
FUEL	C	4.00000	H	6.00000	N	4.00000			.17000	52400.000		298.00	-0.0000
OXIDANT	C	3.00000	H	6.00000	O	6.00000	N	6.00000	.60000	14900.000		298.00	-0.0000
OXIDANT	C	1.00000	H	9.00000	O	3.00000	N	7.00000	.40000	-11590.000		298.00	-0.0000

O/F= 2.3333 PERCENT FUEL= 30.0000 EQUIVALENCE RATIO= 2.6826 DENSITY= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.000	1.826	1.200	1.400	1.600	2.000	3.000	4.000	5.000	10.000	68.000
P, ATM	340.2	186.4	283.5	243.0	212.6	170.1	113.4	85.06	68.05	34.02	5.003
T, CP, DEG K	2051	1795	1970	1904	1848	1759	1610	1517	1451	1285	1019
H, CAL/G	[illegible]	-24.9	58.7	27.1	.6	-42.0	-114.2	-161.6	-196.4	-294.	-513.2
S, CAL/(G)(K)	2.5166	2.5166	2.5166	2.5166	2.5166	2.5166	2.5166	2.5166	2.5166	2.5166	2.5166
M, MOL WT	18.760	18.777	18.763	18.766	18.77	18.783	18.823	18.875	18.934	19.227	20.449
(DLV/DLP)T	-1.00316	-1.00507	-1.00350	-1.00393	-1.00443	-1.00561	-1.00943	-1.01395	-1.01859	-1.03637	-1.07293
(DLV/DLT)P	1.0171	1.0359	1.0207	1.0249	1.0297	1.0412	1.0794	1.1274	1.1795	1.4046	2.1373
CP, CAL/(G)(K)	.4866	.4956	.4871	.4887	.4914	.4995	.5338	.5833	.6413	.9227	2.2581
GAMMA (S)	1.2855	1.2888	1.2871	1.2881	1.2886	1.2886	1.2837	1.2746	1.2644	1.2264	1.1412
SON VEL,M/SEC	1081.0	1012.0	1063.0	1042.3	1027.0	1001.7	955.6	922.7	897.5	825.6	687.6
MACH NUMBER	0.000	1.000	.538	.737	.877	1.079	1.393	1.596	1.747	2.195	3.288
VEL, FT/SEC	0.0	3320.3	1870.0	2518.8	2955.1	3545.2	4366.5	4838.7	5144.8	5944.9	7416.6
VISC, G/CM-SEC	.000624	.000568	.000606	.000592	.000580	.000561	.000528	.000508	.000493	.000460	.000397
L, CAL/G-SEC-K	.000401	.000366	.000390	.000381	.000374	.000361	.000340	.000326	.000316	.000289	.000234
T, CV, DEG K	2637										
IMPETUS	390870.										
CSTAR, FT/SEC		4704	4704	4704	4704	4704	4704	4704	4704	4704	4704
CF		.706	.398	.536	.627	.794	.928	1.027	1.094	1.264	1.577
AE/AT		1.000	1.282	1.073	1.014	1.005	1.118	1.266	1.417	2.139	8.693
IVAC,LB-SEC/LB		183.3	214.3	190.3	184.5	183.7	190.2	196.4	201.3	216.1	249.2
I, LB-SEC/LB		103.2	58.1	78.3	91.8	110.2	135.7	150.1	159.9	184.8	230.5

TABLE XI. Concluded

MOLE FRACTIONS

C(S)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	.02182
CH3	.00001	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	0.00000
CH4	.00055	.00112	.00066	.00079	.00094	.00128	.00239	.00381	.00541	.01327	.03484
CO	.26713	.26459	.26649	.26587	.26527	.26408	.26121	.25841	.25569	.24392	.17825
CO2	.01182	.01421	.01244	.01304	.01360	.01466	.01708	.01927	.02138	.02960	.06425
H	.00007	.00001	.00005	.00003	.00002	.00001	.00000	.00000	.00000	.00000	0.00000
HCN	.00032	.00019	.00027	.00024	.00021	.00017	.00012	.00009	.00006	.00004	.00000
HCO	.00005	.00002	.00004	.00003	.00002	.00001	.00001	.00000	.00000	.00000	.00000
H2	.33571	.33705	.33618	.33654	.33682	.33717	.33707	.33598	.33431	.32430	.26069
H2O	.06992	.06806	.06938	.06890	.06848	.06777	.06659	.06602	.06582	.06659	.07784
NH3	.00069	.00061	.00066	.00064	.00062	.00060	.00057	.00055	.00054	.00047	.00024
N2	.31373	.31414	.31382	.31391	.31401	.31424	.31495	.31585	.31686	.32181	.33488

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CN	CN2	C2	C2H	C2H2	C2H4	C2N
C2N2	C2O	C3	HO2	H2O(L)	H2O(S)	N	NH	NH2	NO
NO2	N2O	N2H4	N2O	N2O4	O	OH	O2		

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

VISCOSITY AND CONDUCTIVITY VALUES BASED ON 99.8 PERCENT OF GAS MIXTURE

TABLE XII. THERMO DATA INPUT FORMAT FOR TITANIUM DIOXIDE

```
 -62000.0   9 51    TITANIUM DIOXIDE (TIO2) IDEAL GAS
298 300 400 500 600 700 800 9001000
 10.838  10.858  11.820  12.548  13.079  13.464  13.746  13.957  14.117
  0.000    .020   1.156   2.376   3.659   4.987   6.348   7.734   9.138
 56.146  56.213  59.474  62.194  64.531  66.578  68.395  70.027  71.506
10001100120013001400150016001700180019002000210022002300240025002600270028002900
30003100320033003400350036003700380039004000410042004300440045004600470048004900
50005100520053005400550056005700580059006000
 14.117  14.[illegible]  14.339  14.417  14.480  14.532  14.575  14.611  14.641  14.667
 14.690  14.709  14.725  14.741  14.754  14.765  14.776  14.785  14.793  14.800
 14.807  14.813  14.819  14.824  14.828  14.832  14.836  14.840  14.843  14.846
 14.849  14.852  14.854  14.856  14.858  14.860  14.862  14.864  14.866  14.867
 14.869  14.870  14.871  14.872  14.874  14.875  14.876  14.877  14.878  14.878
 14.879
  9.138  10.556  11.985  13.423  14.868  16.319  17.774  1[illegible].234  20.696  22.162
 23.630  25.099  26.571  28.045  29.519  30.995  32.472  33.950  35.429  36.909
 38.389  39.870  41.352  42.834  44.317  45.800  47.283  48.767  50.251  51.736
 53.220  54.705  56.191  57.676  59.162  60.648  62.134  63.620  65.107  66.593
 68.080  69.567  71.054  72.541  74.029  75.516  77.004  78.491  79.979  81.467
 82.955
 71.506  72.858  74.101  75.252  76.323  77.324  78.263  79.147  79.948  80.776
 81.529  82.246  82.931  83.586  84.213  84.816  85.395  85.953  86.491  87.010
 87.512  87.997  88.468  88.924  89.336  89.796  90.214  90.621  91.017  91.402
 91.778  92.145  92.503  92.852  93.194  93.528  93.854  94.174  94.487  94.794
 95.094  95.388  95.677  95.960  96.238  96.511  96.779  97.043  97.301  97.556
 97.806
```

TABLE XIII. THERMØ DATA OUTPUT FORMAT FOR TITANIUM DIOXIDE

TITANIUM DIOXIDE (TIO2) IDEAL GAS

HO = -62000.0

VALUES OF G
COEFFICIENTS ARE
.30725340E+01 .10003020E-01 -.11120307E-04 .49403359E-08 -.67934354E-12 -.32508921E+05 .79567663E+01
-.33589155E-02 -.54917462E-02 -.15152376E-01

T	CP	CCP	HT	CHT	ST	CST	DCP	DHT	DST
298.	10.838	10.838	0.000	0.000	56.146	56.146	.006	0.000	.000
300.	10.850	10.866	.020	.022	56.213	56.219	.002	.002	.006
400.	11.820	11.816	1.156	1.158	59.474	59.480	.004	.002	.006
500.	12.548	12.540	2.376	2.377	62.194	62.198	.008	.001	.004
600.	13.079	13.076	3.659	3.659	64.531	64.534	.003	.000	.003
700.	13.464	13.465	4.987	4.987	66.578	66.581	.001	.000	.003
800.	13.746	13.746	6.348	6.349	68.395	68.398	.000	.001	.003
900.	13.957	13.953	7.734	7.734	70.027	70.030	.004	.000	.007
1000.	14.117	14.118	9.138	9.138	71.506	71.509	.001	.000	.003

VALUES OF G
COEFFICIENTS ARE
.62406076E+01 .12846967E-02 -.50184624E-06 .85525393E-10 -.53125222E-14 -.32336518E+05 -.81070897E+01
.95768211E-01 .22837632E-01 .10773479E+00

T	CP	CCP	HT	CHT	ST	CST	DCP	DHT	DST
1000.	14.117	14.117	9.138	9.138	71.506	71.506	.000	.000	.000
1100.	14.241	14.214	10.556	10.555	72.858	72.856	.027	.001	.002
1200.	14.339	14.301	11.985	11.981	74.101	74.097	.038	.004	.004
1300.	14.417	14.379	13.423	13.415	75.252	75.245	.038	.008	.007
1400.	14.480	14.447	14.868	14.856	76.323	76.313	.033	.012	.010
1500.	14.532	14.508	16.319	16.304	77.324	77.312	.024	.015	.012
1600.	14.575	14.561	17.774	17.757	78.263	78.250	.014	.017	.013
1700.	14.611	14.607	19.234	19.216	79.147	79.134	.004	.018	.013
1800.	14.641	14.646	20.696	20.678	79.948	79.970	.005	.018	.022
1900.	14.667	14.681	22.162	22.145	80.776	80.763	.014	.017	.013
2000.	14.690	14.709	23.630	23.614	81.529	81.516	.019	.016	.013
2100.	14.709	14.734	25.099	25.086	82.246	82.235	.025	.013	.011
2200.	14.726	14.754	26.571	26.561	82.931	82.921	.028	.010	.010
2300.	14.741	14.771	28.045	28.037	83.586	83.577	.030	.008	.009
2400.	14.754	14.784	29.519	29.515	84.213	84.206	.030	.004	.007
2500.	14.766	14.796	30.995	30.954	84.816	84.809	.030	.001	.007
2600.	14.776	14.803	32.472	32.474	85.395	85.390	.027	.002	.005
2700.	14.785	14.809	33.950	33.954	85.953	85.949	.024	.004	.004
2800.	14.793	14.814	35.429	35.435	86.491	86.487	.021	.006	.004
2900.	14.800	14.817	36.909	36.917	87.010	87.007	.017	.008	.003
3000.	14.807	14.819	38.389	38.399	87.512	87.510	.012	.010	.002
3100.	14.813	14.821	39.870	39.881	87.997	87.995	.008	.011	.002
3200.	14.819	14.821	41.352	41.363	88.468	88.466	.002	.011	.002
3300.	14.824	14.822	42.834	42.845	88.924	88.922	.002	.011	.002
3400.	14.828	14.823	44.317	44.327	89.336	89.365	.005	.010	.029
3500.	14.832	14.823	45.800	45.810	89.796	89.794	.009	.010	.002
3600.	14.836	14.824	47.283	47.292	90.214	90.212	.012	.009	.002
3700.	14.840	14.825	48.767	48.775	90.621	90.618	.015	.008	.003
3800.	14.843	14.827	50.251	[illegible].257	91.017	91.013	.016	.006	.004
3900.	14.846	14.829	51.736	[illegible]	91.402	91.399	.017	.004	.003
4000.	14.849	14.832	53.220	53.[illegible]	91.778	91.774	.017	.003	.004
4100.	14.852	14.836	54.705	54.706	92.145	92.140	.017	.001	.005
4200.	14.854	14.839	56.191	56.190	92.503	92.498	.015	.001	.005
4300.	14.856	14.844	57.676	57.674	92.852	92.847	.012	.002	.005
4400.	14.858	14.848	59.162	59.159	93.194	93.188	.010	.003	.006
4500.	14.860	14.854	60.647	60.644	93.528	93.522	.006	.007	.006
4600.	14.862	14.859	62.134	62.130	93.854	93.849	.003	.004	.005
4700.	14.864	14.865	63.620	63.616	94.174	94.168	.001	.004	.006
4800.	14.866	14.871	65.107	65.103	94.487	94.481	.005	.004	.006
4900.	14.867	14.876	66.593	66.590	94.794	94.788	.009	.003	.006
5000.	14.869	14.881	68.080	68.078	95.094	95.089	.012	.002	.005
5100.	14.870	14.886	69.567	69.566	95.388	95.383	.016	.001	.005
5200.	14.871	14.889	71.054	71.055	95.677	95.672	.018	.001	.005
5300.	14.872	14.892	72.541	72.544	95.960	95.956	.020	.003	.004
5400.	14.874	14.893	74.029	74.033	96.238	96.235	.019	.004	.003
5500.	14.875	14.892	75.516	75.523	96.511	96.508	.017	.007	.003
5600.	14.876	14.889	77.004	77.012	96.779	96.776	.013	.008	.003
5700.	14.877	14.883	78.491	78.500	97.043	97.040	.006	.009	.003
5800.	14.878	14.875	79.979	79.988	97.301	97.298	.003	.009	.003
5900.	14.878	14.862	81.467	81.475	97.556	97.553	.016	.008	.003
6000.	14.879	14.847	82.955	82.960	97.806	97.802	.032	.005	.004

TABLE XIV. DATA TAPE FORM FOR THERMØ DATA OUTPUT

```
TIO2                J 6/70TI  10   200  000  0G  298.000  6000.000              1
 0.62406876E+01 0.12846967E-02-0.50184624E-06 0.85525393E-10-0.53125222E-14     2
-0.33336518E+05-0.81878897E+01 0.30725348E+01 0.10883020E-01-0.11120307E-04     3
 0.49483359E-08-0.67934354E-12-0.32508921E+05 0.79567663E+01                    4
```

SECTION V

THERMØ DATA PROGRAM

The program (Appendix II) to fit the tabular JANAF thermochemical data to the Lewis polynomial is relatively simple and straightfor ard. JANAF data for Cp, H, and S is read in the tabular form for two temperature ranges 298° to 1,000°K and 1,000° to 6,000°K. The format is as shown in Table XII for the gas TIØ2. The first line consists of the reference heat of formation to 298°K in calories per mole, the number of points in the first temperature range and the number of points in the second temperature range, followed by a species identifier. The tabular temperature references for the first interval are then listed followed by the appropriate Cp, H, and S values. This sequence is then repeated for the second temperature range. Subsequent to data input, the program establishes a matrix which it solves by an inversion procedure to obtain the required polynomial constants. These constants are then output in the form suitable for inclusion on the Lewis program thermodynamic data tape.

The output is as shown on Table XIII for the $TiØ_2$ species which is also shown on the input. The coefficients required on the data card for the first temperature range are shown on the first line followed by a comparison between the tabular data and the generated polynomials for the three functions of interest. It can be seen that the data fit is quite good. These data are followed by the required constants for the second temperature range and a similar comparison of polynomial and tabular results.

These results are read onto the data tape in the form shown on Table XIV. There are four cards per species. The first line consists of the empirical formula in columns 1 to 12. A gaseous species has no subscript, a liquid, has subscript L, and a solid, has subscript S. Columns 19 to 21 contain a code for the data source, in this case, a J for the JANAF tables. Columns 22 to 24 are the month and year of polynomial computation. The first through the fourth atoms in the species are inserted in columns 25 and 26, 30 and 31, 35 and 36, 40 and 41, while the respective number of atoms are placed in columns 27 to 29, 32 to 34, 37 to 39, and 42 to 44. Column 45 is used for the phase of the species G, L, or S. Columns 46 through 55 have the lower temperature bound at which the species exists with the upper temperature bound being placed in columns 56 through 65.

Cards 2, 3, and 4 contain the 14 polynomial constants, five each on cards 2 and 3 and four on card 4.

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APPENDIX I

LEWIS PROGRAM LISTING

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```
      PROGRAM P1712(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE4,TAPE9)    P1712  00002
C                                                                         P1712  00003
C     I C R P G  REFERENCE PROGRAM  ODE                                   P1712  00004
C     DECK SEQUENCED BY SUBROUTINE                                        P1712  00005
C     THERMODYNAMIC DATA FOLLOWS SOURCE DECK                              P1712  00006
C     DATA FOR TEST CASES FOLLOWS THERMODYNAMIC DATA                      P1712  00007
C     PROGRAM USES TAPE UNIT 4 FOR THERMO DATA                            P1712  00008
C                                                                         P1712  00009
C     ODE  ICRPG REFERENCE PROGRAM                                        P1712  00010
C                                                                         P1712  00011
C  MAIN PROGRAM                                                           P1712  00012
C                                                                         P1712  00013
      DOUBLE PRECISION G,X                                                P1712  00014
      INTEGER DATA, OMIT, ENSERT, REAC, BLANK, THRM, END,SUB               P1712  00015
      LOGICAL HP,SP,TP,IDEBUG,NEWR,IONS,MOLES,FROZ,EQL,PSIA,RKT           P1712  00016
      LOGICAL SHOCK,MHHG,PASCAL,EV,IC,DETN,CPCVFR,CPCVEQ,SIUNIT,EUNITS    P1712  00017
C                                                                         P1712  00018
      DIMENSION OMIT(3,3),NCD(4),ENSERT(3,3),LH(2),LVP(2) ,LVM(2)         P1712  00019
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)         P1712  00020
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)    P1712  00021
     2  ,TOTN(13)                                                         P1712  00022
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)     P1712  00023
     1 ,CELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)               P1712  00024
      COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),BOP(15,2)    P1712  00025
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AC(2),AM(2)  P1712  00026
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)           P1712  00027
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)  P1712  00028
     4 ,RHOP,RMW(15),TLN,JANF                                             P1712  00029
      COMMON /DOUBLE/ G(20,21), X(20)                                     P1712  00030
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS,  P1712  00031
     1  KMAT,IMAT,IGI,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ       P1712  00032
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                     P1712  00033
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)  P1712  00034
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSO                               P1712  00035
C                                                                         P1712  00036
      EQUIVALENCE (OMIT,ENLN),(ENSERT,EN(1,3))                            P1712  00037
C                                                                         P1712  00038
      DATA MIT/4HOMIT/,BLANK/1H /, PSIA/4HPSIA/,REAC/4HREAC/,             P1712  00039
     1   INPUT/4HINPU/,IE/1HE/,INSERT/4HINSE/,THRM/4HTHER/,END/3HEND/     P1712  00040
      DATA LH/4HH,CA,4HL/G /,LVP/2HV+,1H /,LVM/2HV-,1H /,NMLT/4HNAME/     P1712  00041
C                                                                         P1712  00042
      NAMELIST/INPT2/JANF,P,T,EQRAT,OF,FPCT,FA,TP,HP,SP,RKT               P1712  00043
     1,PSIA,MHHG,SHOCK,IONS,EV,V,DETN,CPCVFR,CPCVEQ,IDEBUG                P1712  00044
     2,SIUNIT,EUNITS                                                      P1712  00045
C                                                                         P1712  00046
      TLOW = 0.                                                           P1712  00047
      NEWR = .FALSE.                                                      P1712  00048
      DO 399 I=1,15                                                       P1712  00049
      DO 398 J=1,150                                                      P1712  00050
      A(I,J) = 0.0                                                        P1712  00051
  398 CONTINUE                                                            P1712  00052
  399 CONTINUE                                                            P1712  00053
C                                                                         P1712  00054
```

```
    1 WRITE(6,400)                                                         P1712 00055
  400 FORMAT(1H1)                                                          P1712 00056
      READ(5,1204) NREAC,NCASE,NSRT,NMIT                                   P1712 00057
 1204 FORMAT(4I3)                                                          P1712 00058
      IF(NREAC.LE.0.OR.NCASE.LE.0) WRITE(6,1023) NREAC,NCASE              P1712 00059
 1023 FORMAT(1H ,*NO REACTANTS OR NO CASES SPECIFIED ON TYPE 1 DATA CARD P1712 00060
     1, NREAC =*,I3,*  NCASE=*,I3)                                        P1712 00061
   11 NOMIT = 0                                                            P1712 00062
      NSERT = 0                                                            P1712 00063
      MOLES = .FALSE.                                                      P1712 00064
      CALL REACT                                                           P1712 00065
      IF(L.EQ.0)  WRITE(6,52)                                              P1712 00066
   52 FORMAT(25H0ERROR IN REACTANT CARDS)                                  P1712 00067
C                                                                          P1712 00068
C     CHECK INSERT CARDS                                                   P1712 00069
C                                                                          P1712 00070
      IF(NSRT.LE.0) GO TO 205                                              P1712 00071
  180 DO 185 K=1,NSRT                                                      P1712 00072
      READ(5,204) (DATA(J),J=1,15)                                         P1712 00073
      WRITE(6,2045) (DATA(J),J=1,15)                                       P1712 00074
  204 FORMAT(5(3A4,3X))                                                    P1712 00075
 2045 FORMAT(1X,5(3A4,3X))                                                 P1712 00076
      DO 185 I=1,15,3                                                      P1712 00077
      IF (DATA(I).EQ.BLANK) GO TO 185                                      P1712 00078
      NSERT = NSERT+1                                                      P1712 00079
      ENSERT(1,NSERT) = DATA(I)                                            P1712 00080
      ENSERT(2,NSERT) = DATA(I+1)                                          P1712 00081
      ENSERT(3,NSERT) = DATA(I+2)                                          P1712 00082
  185 CONTINUE                                                             P1712 00083
C                                                                          P1712 00084
C     CHECK OMIT CARDS                                                     P1712 00085
C                                                                          P1712 00086
  205 IF(NMIT.LE.0) GO TO 210                                              P1712 00087
      DO 208 K=1,NMIT                                                      P1712 00088
      READ(5,204) (DATA(J),J=1,15)                                         P1712 00089
      WRITE(6,2045) (DATA(J),J=1,15)                                       P1712 00090
      DO 208 I=1,15,3                                                      P1712 00091
      IF(DATA(I).EQ.BLANK) GO TO 208                                       P1712 00092
      NOMIT = NOMIT+1                                                      P1712 00093
      OMIT(1,NOMIT) = DATA(I)                                              P1712 00094
      OMIT(2,NOMIT) = DATA(I+1)                                            P1712 00095
      OMIT(3,NOMIT) = DATA(I+2)                                            P1712 00096
  208 CONTINUE                                                             P1712 00097
      NEWR= .TRUE.                                                         P1712 00098
C                                                                          P1712 00099
C     BEGIN NAMELIST INPT2                                                 P1712 00100
C                                                                          P1712 00101
  210 DO 500 NCS=1,NCASE                                                   P1712 00102
      DO 300 I=1,26                                                        P1712 00103
      OCP(I) = 0.                                                          P1712 00104
      P(I)= 0.                                                             P1712 00105
      T(I)= 0.                                                             P1712 00106
      V(I) = 0.                                                            P1712 00107
```

```
  300 CONTINUE
      V1 = 0.
      V2 = 0.
      RHOP = 0.
      KASE= 0
      TP = .FALSE.
      HP=.FALSE.
      SP=.FALSE.
      RKT = .FALSE.
      CPCVFR = .FALSE.
      CPCVEQ = .FALSE.
      SHOCK = .FALSE.
      DETN = .FALSE.
      EV = .FALSE.
      PASCAL = .FALSE.
      MMHG   = .FALSE.
      PSIA = .FALSE.
      R = 1.987165
      RR = 4184.*R
      SIUNIT = .FALSE.
      EUNITS = .FALSE.
      IONS = .FALSE.
      IDEBUG=.FALSE.
      FA = 0.
      OF = 0.
      EQRAT= 0.
      FPCT= 0.
      EQL = .TRUE.
      READ(5,303)KASE
  303 FORMAT(13A6,A2)
      READ(5,INPT2)
      DO 305 I=1,26
      IF(P(I ).EQ.0.) GO TO 322
      NP = I
      IF (MMHG) P(NP) = P(NP)/760.
      IF (PASCAL) P(NP) = P(NP)/101325.
      IF(PSIA       )  P(NP)=P(NP)/14.696006
  305 CONTINUE
  322 IF (FA.NE.0.) OF = 1./FA
      IF(EQRAT.EQ.0.) GO TO 725
      OF= (-EQRAT*VMIN(2)-VPLS(2))/(VPLS(1)+EQRAT*VMIN(1))
      GO TO 727
  725 IF(OF.NE.0.) GO TO 727
      IF(FPCT.EQ.0.) GO TO 9051
      OF= (100.-FPCT)/FPCT
      GO TO 727
 9051 WRITE(6,724)
  724 FORMAT(48HONO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT  )
      IF(WP(2).NE.1.) OF=WP(1)/WP(2)
  727 WP(1) = OF
      WP(2) = 1.
      SUM = WP(1)+WP(2)
      FPCT = 100.*WP(2)/SUM
```

```
      IF (EQRAT.NE.0.)  GO TO 746
      V2 = (WP(1)*VMIN(1)+WP(2)*VMIN(2))/SUM
      V1 = (WP(1)*VPLS(1)+WP(2)*VPLS(2))/SUM
      IF(V2.NE.0.)  EQRAT=ABS(V1/V2)
  746 DO 747 I=1,L
      BO(I) = (WP(1)*BOP(I,1)+WP(2)*BOP(I,2))/SUM
  747 CONTINUE
      IF (EQRAT.EQ.1.)  EQRAT= 1.000005
      IF(.NOT.IONS.OR.LLMT(L).EQ.IE)  GO TO 748
      L = L+1
      LLMT(L) = IE
      BO(L) = 0.
  748 HSUBO = (WP(1)*HPP(1)+WP(2)*HPP(2))/SUM
      WRITE (6,INPT2)
      WRITE(6,752)KASE
  752 FORMAT(1H0,13A6,A2/)
      WRITE (6,770)
  770 FORMAT (1H0,17X,4HFUEL ,13X,7HOXIDANT  ,12X,7HMIXTURE   //)
  780 FORMAT (1H 2A4,3E15.8/)
      WRITE (6,780) LH,HPP(2),HPP(1),HSUBO,LVP,VPLS(2),VPLS(1),V1,
     1LVM,VMIN(2),VMIN(1),V2
      HSUBO = HSUBO/R
      WRITE (6,785)
  785 FORMAT (8H ATOMS/G  )
      WRITE(6,780)(LLMT(I),BLANK,BOP(I,2),BOP(I,1),BO(I),I=1,L)
      RHOP = WP(2)*RHO(1)+WP(1)*RHO(2)
      IF(RHOP.NE.0.)  RHOP = (WP(1)+WP(2))*RHO(1)*RHO(2)/RHOP
  786 IF(NEWR) CALL SEARCH
      IQ1= L+1
      IF(NC.EQ.0)  GO TO 790
      DO 302 J=1,NS
      IF(IUSE(J).EQ.0) GO TO 302
      IF(IUSE(J).GT.0) IUSE(J)= -IUSE(J)
      IF(NSERT.EQ.0) GO TO 302
      DO 301 I=1,NSERT
      IF(SUB(J,1).NE.ENSERT(1,I)) GO TO 301
      IF(SUB(J,2).NE.ENSERT(2,I)) GO TO 301
      IF(SUB(J,3).NE.ENSERT(3,I)) GO TO 301
      ENSERT(1,I) =0.
      IQ1= IQ1+1
      IUSE(J)= -IUSE(J)
  301 CONTINUE
  302 CONTINUE
      NSERT = 0
  790 ITN= 35
      IC = .FALSE.
      PP = NS
      NPT = 1
      ENN = .1
      SUMN = ENN
      XI = NS - NC
      XI = ENN/XI
      XLN = ALOG(XI)
```

```
      DO 432 J=1,NS                                   P1712  00214
      IF(IUSE(J).EQ.-10000)  IUSE(J)=0                P1712  00215
      EN(J,1) = 0.                                    P1712  00216
      ENLN(J)=0.                                      P1712  00217
      IF (IUSE(J).NE.0)  GO TO 432                    P1712  00218
      EN(J,1) = XI                                    P1712  00219
      ENLN(J) = XLN                                   P1712  00220
  432 CONTINUE                                        P1712  00221
      JSCL = 0                                        P1712  00222
      JLIQ = 0                                        P1712  00223
      IF(DETN) CALL DETON                             P1712  00224
      IF(RKT) CALL ROCKET                             P1712  00225
      IF (TP) CALL MOLIER                             P1712  00226
      IF(HP) CALL CMBSTN                              P1712  00227
  500 CONTINUE                                        P1712  00228
      GO TO 1                                         P1712  00229
      END                                             P1712  00230
```

```
      BLOCK DATA                                                          P1712   00231
C                                                                         P1712   00232
      DIMENSION ATEM(3,53)                                                P1712   00233
C                                                                         P1712   00234
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)    P1712   00235
     1 ,TM,TLOW,TMIG,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)  P1712   00236
     2 ,HPP(2),HO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)            P1712   00237
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)  P1712   00238
     4 ,RHOP,RMW(15),TLN,JANF                                             P1712   00239
      COMMON/OUPT/FMT(39),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)       P1712   00240
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),F4TI9,FA1,FA2          P1712   00241
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0                         P1712   00242
C                                                                         P1712   00243
      EQUIVALENCE (ATOM(1,52),ATEM)                                       P1712   00244
C                                                                         P1712   00245
C  ATOMIC SYMBOLS, WEIGHTS, AND VALENCES                                  P1712   00246
C                                                                         P1712   00247
      DATA ((ATOM(I,J),I=1,3),J=1,25)/                                    P1712   00248
     A    2HH ,  1.008, 1.,   2HHE,  4.003, 0.,   2HLI,  6.940, 1.,       P1712   00249
     B    2HBE,  9.013, 2.,   2HB , 10.820, 3.,   2HC , 12.011, 4.,       P1712   00250
     C    2HN , 14.008, 0.,   2HO , 16.000,-2.,   2HF , 19.000,-1.,       P1712   00251
     D    2HNE, 20.183, 0.,   2HNA, 22.991, 1.,   2HMG, 24.320, 2.,       P1712   00252
     E    2HAL, 26.980, 3.,   2HSI, 28.090, 4.,   2HP , 30.975, 5.,       P1712   00253
     F    2HS , 32.066, 4.,   2HCL, 35.457,-1.,   2HAR, 39.944, 0.,       P1712   00254
     G    2HK , 39.100, 1.,   2HCA, 40.080, 2.,   2HSC, 44.960, 3.,       P1712   00255
     H    2HTI, 47.930, 4.,   2HV , 50.950, 5.,   2HCR, 52.010, 3.,       P1712   00256
     I  2HMN,54.940,2./                                                   P1712   00257
      DATA ((ATOM(I,J),I=1,3),J=26,51)/                                   P1712   00258
     I  2HFE,55.850,3.,  2HCO,58.940,2.,                                  P1712   00259
     J    2HNI, 58.710, 2.,   2HCU, 63.540, 2.,   2HZN, 65.380, 2.,       P1712   00260
     K    2HGA, 69.720, 3.,   2HGE, 72.600, 4.,   2HAS, 74.920, 3.,       P1712   00261
     L    2HSE, 78.960, 4.,   2HBR, 79.916,-1.,   2HKR, 83.800, 0.,       P1712   00262
     M    2HRB, 85.480, 1.,   2HSR, 87.630, 2.,   2HY , 88.910, 3.,       P1712   00263
     N    2HZR, 91.220, 4.,   2HNB, 92.910, 5.,   2HMO, 95.950, 6.,       P1712   00264
     O    2HTC, 99.000, 7.,   2HRU,101.100, 3.,   2HRH,102.910, 3.,       P1712   00265
     P    2HPD,106.400, 2.,   2HAG,107.880, 1.,   2HCD,112.410, 2.,       P1712   00266
     Q    2HIN,114.820, 3.,   2HSN,118.700, 4.,   2HSB,121.760, 3./       P1712   00267
      DATA ATEM/                                                          P1712   00268
     R    2HTE,127.610, 4.,   2HI ,126.910,-1.,   2HXE,131.300, 0.,       P1712   00269
     S    2HCS,132.910, 1.,   2HBA,137.360, 2.,   2HLA,138.920, 3.,       P1712   00270
     T    2HCE,140.130, 3.,   2HPR,140.910, 3.,   2HND,144.270, 3.,       P1712   00271
     U    2HPM,147.000, 3.,   2HSM,150.350, 3.,   2HEU,152.000, 3.,       P1712   00272
     V    2HGD,157.260, 3.,   2HTB,158.930, 3.,   2HDY,162.510, 3.,       P1712   00273
     W    2HHO,164.940, 3.,   2HER,167.270, 3.,   2HTM,168.940, 3.,       P1712   00274
     X    2HYB,173.040, 3.,   2HLU,174.990, 3.,   2HHF,178.500, 4.,       P1712   00275
     Y    2HTA,180.950, 5.,   2HW ,183.860, 6.,   2HRE,186.220, 7.,       P1712   00276
     Z    2HOS,190.200, 4.,   2HIR,192.200, 4.,   2HPT,195.090, 4.,       P1712   00277
     A    2HAU,197.000, 3.,   2HHG,200.610, 2.,   2HTL,204.390, 1.,       P1712   00278
     B    2HPB,207.210, 2.,   2HBI,209.000, 3.,   2HPO,210.000, 2.,       P1712   00279
     C    2HAT,210.000, 0.,   2HRN,222.000, 0.,   2HFR,223.000, 1.,       P1712   00280
     D    2HRA,226.000, 2.,   2HAC,227.000, 3.,   2HTH,232.000, 4.,       P1712   00281
     E    2HPA,231.000, 5.,   2HU ,238.000, 6.,   2HNP,237.000, 5.,       P1712   00282
     F    2HPU,242.000, 4.,   2HAM,243.000, 3.,   2HCM,247.000, 3.,       P1712   00283
```

```
       G    2HBK,249.000, 3.,   2HCF,251.000, 3.,   2HES,254.000, 0.,   P1712  00284
       H    2HFM,253.000, 0.,   2HMV,256.000, 0./                       P1712  00285
C                                                                       P1712  00286
C      INFORMATION USED IN VARIABLE OUTPUT FORMAT                       P1712  00287
C                                                                       P1712  00288
       DATA FMT/34(1H,4H,3A4,4H,A2,,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1 P1712  00289
      1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF P1712  00290
      29.,1H ,3HF9.,1H ,3HF9.,1H ,1H)/, F8,F0,F1,F2,F3,F4,F5/1H  ,2H0,,2H P1712  00291
      31,,2H2,,2H3,,2H4,,2H5,/,FMT13/2H13/,FMT9X/3H9X,/,FMTI9/3HI9,/     P1712  00292
       DATA                          FP/4HP, A,4HTM  ,2H  ,1H /          P1712  00293
      1,FT/4HT, C,4HP, D,4HEG K,2H  /,FH/4HH, C,4HAL/G,2H  ,1H /          P1712  00294
      2,FS/4HS, C,4HAL/(,4HG)(K,2H) /,FM/4HM, M,4HOL W,2HT ,1H /          P1712  00295
      3,FV/4H(DLV,4H/DLP,4H)T  ,2H  /,FD/4H(DLV,4H/DLT,2H)P,1H /          P1712  00296
      4,FC/4HCP, ,4HCAL/,4H(G)(,2HK)/,FG/4HGAMM,4HA (S,2H) ,1H /          P1712  00297
      5,FL/4HSON ,4HVEL,,4HM/SE,2HC /                                    P1712  00298
C                                                                       P1712  00299
C      INFORMATION USED IN PERFORMANCE OUTPUT                           P1712  00300
C                                                                       P1712  00301
       DATA FR1/4HPC/P/, FC1/2HCF/,    FN/4HMACH,4H NUM,4HBER ,1H /      P1712  00302
      1,FR/4HCSTA,4HR, F,4HT/SE,2HC  /,FI/4HI, L,4HB-SE,4HC/LB,1H /      P1712  00303
      2,FA/4HIVAC,4H,LB-,4HSEC/,2HLB /,FA1/4HAE/A/,FA2/1HT/             P1712  00304
       END                                                              P1712  00305
```

```
      SUBROUTINE CMBSTN                                                  P1712  00306
C                                                                        P1712  00307
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)        P1712  00308
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),[illegible](13),SONVEL(13),TTT(13)  P1712  00309
     2,TCTN(13)                                                          P1712  00310
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)   P1712  00311
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)             P1712  00312
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)  P1712  00313
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712  00314
     2 ,HPP(2),RH0(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)         P1712  00315
     3 ,ANUM(15,5),PECWT(15),CNTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  00316
     4 ,RHOP,RAW(15),TLN,JANF                                            P1712  00317
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  00318
     1  KMAT,IMAT,IC1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ      P1712  00319
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                   P1712  00320
C                                                                        P1712  00321
C     SET ASSIGNED P                                                     P1712  00322
C                                                                        P1712  00323
      TT = 3800.                                                         P1712  00324
      DO 902 IP = 1,NP                                                   P1712  00325
      PP = P(IP)                                                         P1712  00326
      CALL EQLBRM                                                        P1712  00327
      T(NPT) = TT                                                        P1712  00328
      IF(TT.NE.0.)  GO TO 800                                            P1712  00329
      IF(NPT.EQ.0)  GO TO 1000                                           P1712  00330
  800 K=0                                                                P1712  00331
      IF(IP.EQ.NP.OR.TT.EQ.0.)  GO TO 860                                P1712  00332
      K = NPT                                                            P1712  00333
      IF(NPT.NE.13)  GO TO 870                                           P1712  00334
  860 WRITE (6,6)                                                        P1712  00335
    6 FORMAT (1H1,42X,48HTHEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES P1712  00336
     1   ///)                                                            P1712  00337
      CALL OUT1                                                          P1712  00338
      WRITE (6,863)                                                      P1712  00339
  863 FORMAT (25H0THERMODYNAMIC PROPERTIES//)                            P1712  00340
      CALL OUT2                                                          P1712  00341
      CALL OUT3                                                          P1712  00342
  865 IF(K.EQ.0) GO TO 1000                                              P1712  00343
      NPT = 0                                                            P1712  00344
  870 NPT = NPT + 1                                                      P1712  00345
C                                                                        P1712  00346
C                                                                        P1712  00347
C     SAVE    POSITIONS FOR ESTIMATES OF NEXT POINT                      P1712  00348
      DO     I = 1,NS                                                    P1712  00349
      EN(I,NPT) = EN(I,K)                                                P1712  00350
  880 CONTINUE                                                           P1712  00351
  902 CONTINUE                                                           P1712  00352
 1000 RETURN                                                             P1712  00353
      END                                                                P1712  00354
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      C                                                                      P1712  00355
            SUBROUTINE CPHS                                                  P1712  00356
            COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)  P1712  00357
           1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)            P1712  00358
            COMMON/ TSC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),BU(15),BOP(15,2) P1712  00359
           1 ,TM, .OW,TMID,THIGH,PP,CPSUM,OF,EQRA),FPCT,R,RR,HSUB0,AC(2),AM(2) P1712  0036C
           2 ,FPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)        P1712  00361
           3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  00362
           4 ,RHOP,RMW(15),TLN,JANF                                          P1712  00363
            COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  00364
           1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ    P1712  00365
           2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                  P1712  00366
      C                                                                      P1712  00367
            K = 1                                                            P1712  00368
            IF(TT.LE.TMID)K = 2                                              P1712  00369
            KK = 0                                                           P1712  00370
            CPSUM=0.                                                         P1712  00371
         90 IF(COEF(K,1,J).NE.0.)GO TO 97                                    P1712  00372
            IF (IUSE(J).LT.0) GO TO 100                                      P1712  00373
            KK = K                                                           P1712  00374
            K = 1                                                            P1712  00375
            IF (KK.EQ.1) K = 2                                               P1712  00376
         97 CONTINUE                                                         P1712  00377
            IF(JANF.EQ. 0)GO TO 98                                           P1712  00378
            S(J)=COEF(K,1,J)*TLN+COEF(K,7,J)-COEF(K,5,J)/2./TT/TT            P1712  00379
           1+((COEF(K,4,J)/3.0*TT+COEF(K,3,J)/2.0)*TT+COEF(K,2,J))*TT        P1712  00380
            H0(J)=(((COEF(K,4,J)/4.0)*TT+COEF(K,3,J)/3.0)*TT+COEF(K,2,J)/2.0)* P1712  00381
           1TT+COEF(K,1,J)-(COEF(K,5,J)/TT-COEF(K,6,J))/TT                   P1712  00382
            CPSUM=CPSUM  ((COEF(K,4,J)*TT+COEF(K,3,J))*TT+COEF(K,2,J))*TT    P1712  00383
           1+COEF(K,1,J -COEF(K,5,J)/TT/TT)*EN(J,NPT)                        P1712  00384
            GO TO 99                                                         P1712  00385
         98 S(J) =  ((((COEF(K,5,J)/4.)*TT+ COEF(K,4,J)/3.)*TT+ COEF(K,3,J)/2. P1712  00386
           1)* TT+COEF(K,2,J))*TT+ COEF(K,1,J)*TLN + COEF(K,7,J)             P1712  00387
            H0(J) = ((((COEF(K,5,J)/5.)*TT+ COEF(K,4,J)/4.)*TT+ COEF(K,3,J)/3. P1712  00388
           1  ) *TT+ COEF(K,2,J)/2.)*TT+ COEF(K,1,J) + COEF(K,6,J)/TT        P1712  00389
            CPSUM= CPSUM+((((COEF(K,5,J)*TT+ COEF(K,4,J))*TT+ COEF  ,3,J))*TT P1712  00390
           1     + COEF(K,2,J))*TT+ COEF(K,1,J))*EN(J,NPT)                   P1712  00391
         99 CONTINUE                                                         P1712  00392
            IF (KK.EQ.0) GO TO 100                                           P1712  00393
            K = KK                                                           P1712  00394
            KK = 0                                                           P1712  00395
        100 IF(J.EQ.NS) GO TO 200                                            P1712  00396
            J=J+1                                                            P1712  00397
            GO TO 90                                                         P1712  00398
        200 RETURN                                                           P1712  00399
            END                                                              P1712  00400
```

```
      SUBROUTINE DETON
C
C
C     CHAPMAN-JOUGUET DETONATIONS
C
      LOGICAL HP,SP,TP,IDEBUG,NEWR,IONS,MOLES,FROZ,EQL,PSIA,RKT
      LOGICAL CPCVEQ, CPCVFR, CALCH
C
      DIMENSION GM(13),CP(13),H1(13),PUB(13),TUB(13),GM1(13),RRHO(13)
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2 ,TOTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,CELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EGRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN,JANF
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS,
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSU
      COMMON/CUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FO(4)
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
C
      EQUIVALENCE(CP,DATA),(GM,SPIM),(H1,VAC1),(PUB,SUBAR),(TUB,SUPAR)
      EQUIVALENCE(GM1,AEAT),(PCP(14),RRHO)
C
      DATA FT1/4HT1,0/, FP1/4HP1,A/, FH1/4HH1,C/, FM1/4HH1,M/
     1 ,  FCP1/4HCP1,/, FG1/4HA1  /, FPP/4HP/P1/, FTT/4HT/T1/
     2 ,   FUD/4HDET /, FMM/4HM/M1/, FRA/4HRHO//, FRE/4HRHO1/
     3 ,   FMA/4HMACH/, FMB/4H NO./, IZERO/2H00/
C
      D(C)= A11*A22-A21*A12
      XX(Y)=  (B1*A22-B2*A12)/D(C)
      YY(Z)=  (B2*A11-B1*A21)/D(C)
C
      NT = 1
      HSUB0 = HSUB0*R
      CALCH=.TRUE.
      TT = 0.
      IF(T(1).EQ.0.)  T(1)=RTEMP(1)
      DO 2 N = 1,NREAC
      IF(NAME(N,5).EQ.IZERO) CALCH = .TRUE.
    2 CONTINUE
      DO 3  IT = 1,26
      IF (T(IT).EQ.0.)  GO TO 7
      NT = IT
    3 CONTINUE
```

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SUBROUTINE  DETON    FORTRAN EXTENDED VERSION 2.0          31/12/70          08.09.56.                PAGE NO.   2

        7 IF (AM(1).NE.0.0 .AND. AM(2).NE.0.0) GO TO 4                    P1712    00454
          AM1 = AM(2)                                                     P1712    00455
          IF (AM(2).EQ.0.0)AM1 = AM(1)                                    P1712    00456
          GC TO 9                                                         P1712    00457
        4 AM1 = (WP(1)+WP(2))*AM(1)*AM(2)/(WP(2)*AM(1)+WF(1)*AM(2))       P1712    00458
    9     CONTINUE                                                        P1712    00459
          DO 902 IT=1,NT                                                  P1712    00460
          T1= T(IT)                                                       P1712    00461
          TT = T1                                                         P1712    00462
          IF (CALCH) CALL HCALC                                           P1712    00463
          CP1 = (WP(1)*AC(1)+WP(2)*AC(2))/(WP(1)+WP(2))                   P1712    00464
          DO 902 IP=1,NP                                                  P1712    00465
          P1= P(IP)                                                       P1712    00466
          H1(NPT) = HSUB0                                                 P1712    00467
          TUB(NPT)=T1                                                     P1712    00468
          PUR(NPT)=P1                                                     P1712    00469
          CP(NPT) = CP1*R                                                 P1712    00470
          ITR= 0                                                          P1712    00471
          TT= 3800.                                                       P1712    00472
          PP1= 15.                                                        P1712    00473
          PP= PP1*P1                                                      P1712    00474
          HSUB0 = H1(NPT)/R + .75*T1*PP1/AM1                              P1712    00475
          TP = .FALSE.                                                    P1712    00476
          HP= .TRUE.                                                      P1712    00477
          CALL EQLBRM                                                     P1712    00478
          HSUB0 = H1(NPT)                                                 P1712    00479
          HP= .FALSE.                                                     P1712    00480
          IF(TT.EQ.0.) GO TO 1000                                         P1712    00481
          GAM= GAMMAS(NPT)                                                P1712    00482
          TT1= TT/T1                                                      P1712    00483
          II= 0                                                           P1712    00484
          TEM=TT1-.75*PP1/(CPR(NPT)*AM1)                                  P1712    00485
          AMM=WM(NPT)/AM1                                                 P1712    00486
          IF(IDEBUG) WRITE(6,190)                                         P1712    00487
      190 FORMAT(33H1DETONATION VELOCITY CALCULATIONS /11X,4HP/P1,17X,4HT/T1 P1712 00488
         1)                                                               P1712    00489
          IF(IDEBUG) WRITE(6,203) II,PP1,TT1                              P1712    00490
    C                                                                     P1712    00491
      200 DO 202 II=1,4                                                   P1712    00492
          ALFA=AMM/TT1                                                    P1712    00493
          PP1= (1.+GAM)*(1.+(1.-4.*GAM*ALFA/(1.+GAM)**2)**.5)/(2.*GAM*ALFA) P1712  00494
          RK=PP1*ALFA                                                     P1712    00495
          TT1= TEM+.5*PP1*GAM*(RK*RK-1.)/(AM1*CPR(NPT)*RK)                P1712    00496
          IF(IDEBUG) WRITE(6,203) II,PP1,TT1                              P1712    00497
      203 FORMAT (I5,2E20.8)                                              P1712    00498
      202 CONTINUE                                                        P1712    00499
          TP= .TRUE.                                                      P1712    00500
          TT= T1*TT1                                                      P1712    00501
          RR1 = PP1*AMM/TT1                                               P1712    00502
    C                                                                     P1712    00503
      205 ITR= ITR+1                                                      P1712    00504
          PP= P1*PP1                                                      P1712    00505
          CALL EQLBRM                                                     P1712    00506
```

```
      IF (NPT.EQ.0) GO TO 1000
      IF (TT.EQ.0.) GO TO 860
      GAM= GAMMAS(NPT)
C     IF(CPCVFR)GAM= CPRF(NPT)/(CPRF(NPT)-1./WM(NPT))
C     IF(CPCVEQ)GAM= -GAMMAS(NPT)*DLVPT(NPT)
      AMM= WM(NPT)/AM1
      RR1= PP1*AMM/TT1
      A11= 1./PP1 + GAM*RR1*DLVPT(NPT)
      A12= GAM*RR1*DLVTP(NPT)
      A21= .5*GAM*(RR1**2-1.-DLVPT(NPT)*(1.+RR1**2))+DLVTP(NPT)-1.
      A22=-.5*GAM*DLVTP(NPT)*(RR1**2+1.)-WM(NPT)*CPR(NPT)
      B1= 1./PP1-1.+GAM*(RR1-1.)
      B2= WM(NPT)*(HSUM(NPT)-H1(NPT)/R)/TT-.5*GAM*(RR1*RR1-1.)
      X1 = XX(Y)
      X2 = YY(Z)
      ALAM= 1.
      TEM = X1
      IF(TEM.LT.0.)  TEM = -TEM
      IF(X2.GT.TEM)  TEM=X2
      IF (-X2.GT.TEM) TEM = -X2
      IF(TEM.GT.0.4) ALAM=.4/TEM
      PP1= PP1*EXP(X1*ALAM)
      TT1= TT1*EXP(X2*ALAM)
      TT = T1*TT1
      US = (RR*GAM*TT/WM(NPT))**.5
      UD= RR1*US
      IF(IDEBUG) WRITE(6,10) ITR
   10 FORMAT (21H0   ITERATION NUMBER=I2        )
      IF(IDEBUG) WRITE(6,30) PP1,TT1,RR1,X1,X2,US
   30 FORMAT(6X,4HP/P1,10X,1H= E20.8/6X,4HT/T1,10X,1H= E20.8/6X,8HRHO/RH
     101,6X,1H= E20.8/6X,11HDEL LN P/P1,3X,1H=E20.8/6X,11HDEL LN T/T1,3X
     2,1H=E20.8/6X,2HUS,12X,1H=E20.8)
C
C     CONVERGENCE TEST
C
      IF(ITR.LE.10 .AND. TEM.GT.0.5E-04)  GO TO 205
      RRHO(NPT)=RR1
      IF (CP(NPT).EQ.0.) GO TO 40
      GM1(NPT) = CP(NPT) /(CP(NPT)-R/AM1)
      VMOC(NPT) = UD/(RR*GM1(NPT)*T1/AM1)**.5
      GO TO 41
   40 GM1(NPT) = 0.
      VMOC(NPT) = 0.
      GO TO 159
C
C    DERIVATIVES
C
   41 IF(IDEBUG) WRITE(6,55)
   55 FORMAT (17H0   DERIVATIVE OF,13X,4HLN P,16X,4HLN T,16X,2HUD,
     1          /9X,2HBY )
      B1= 1./PP1-GAM*RR1
      B2= GAM*RR1**2
      X1 = XX(Y)
```

```
      X2 = YY(Z)
      AA= .5*(1.-DLVPT(NPT))
      BB= -.5*DLVTP(NPT)
      DUC= UD*(AA*X1+BB*X2-1.)
      X1= X1-1.0
      IF(IDEBUG) WRITE(6,81) X1,X2,DUD
   81 FORMAT(6X,13HLNP1 AT T1,H1,GX,1H=,3E17.8)
      B1= GAM*RR1
      B2= -B1*RR1-WM(NPT)*CP(NPT)/(R*TT1)
      X1 = XX(Y)
      X2 = YY(Z)
      DUD= UD*(AA*X1+BB*X2+1.)
      X2= X2-1.
      IF(IDEBUG) WRITE(6,84) X1,X2,DUD
   84 FORMAT(6X,16HLNT1 AT P1,H1,M1,3X,1H=3E17.8)
      B1= 0.
      B2= -WM(NPT)/(R*TT)
      X1 = XX(Y)*1000.
      X2 = YY(Z)*1000.
      DUD= UD*(AA*X1+BB*X2)
      IF(IDEBUG) WRITE(6,85) X1,X2,DUD
   85 FORMAT (6X,20HH1    AT T1,P1,H1    =3E17.8)
C
  150 K = 0
      IF(IP.EQ.NP.AND.IT.EQ.NT.OR.TT.EQ.0.)  GO TO 860
      K = NPT
      IF(NPT.NE.13)  GO TO 870
C
C  OUTPUT
C
  860 WRITE (6,5)
    5 FORMAT(1H1,42X,46HDETONATION PROPERTIES OF AN IDEAL REACTING GAS )
      CALL OUT1
      WRITE(6,46)
   46 FORMAT(13H UNBURNED GAS//)
      FMT(4)=FMT13
      FMT(5)=F8
      FMT(7)=F4
      WRITE(6,FMT)FP1,FP(2),F8,F8,(PUB(J),J=1,NPT)
      FMT(7)=F2
      WRITE(6,FMT)FT1,FT(2),F8,F3,(TUB(J),J=1,NPT)
      WRITE(6,FMT)FH1,FH(2),F8,F8,(H1(J), J=1,NPT)
      DO 56 I=1,NPT
      V(I)=AM1
      SONVEL(I)=     (RR*GM1(I)*TUB(I)/AM1)**.5
   56 CONTINUE
      FMT(7)=F3
      WRITE(6,FMT)  FM1,FM(2),FM(3),F8,(V(J),J=1,NPT)
      FMT(7)=F4
      WRITE(6,FMT)FCP1,FC(2),FC(3),FC(4),(CP(J),J=1,NPT)
      WRITE(6,FMT)FG(1),FG1,F8,F8,(GM1(J),J=1,NPT)
      FMT(7)=F1
      WRITE(6,FMT)(FL(I),I=1,4),(SONVEL(J),J=1,NPT)
```

```
      WRITE(6,58)                                                      P1712  00613
   58 FORMAT(11H0BURNED GAS//)                                         P1712  00614
      FMT(4)=FMT(6)                                                    P1712  00615
      CALL OUT2                                                        P1712  00616
      WRITE(6,68)                                                      P1712  00617
   68 FORMAT(22H0DETONATION PARAMETERS //)                             P1712  00618
      FMT(7)=F3                                                        P1712  00619
      DO 70 I=1,NPT                                                    P1712  00620
      V(I)= PPP(I)/PUB(I)                                              P1712  00621
      PCP(I)=TTT(I)/TUB(I)                                             P1712  00622
      SONVEL(I)=SONVEL(I)*RRHO(I)                                      P1712  00623
   70 CONTINUE                                                         P1712  00624
      WRITE(6,FMT)FPP,FB,FB,FB,(V(J),J=1,NPT)                          P1712  00625
      WRITE(6,FMT)FTT,FB,FB,FB,(PCP(J),J=1,NPT)                        P1712  00626
      DO 73 I=1,NPT                                                    P1712  00627
      V(I)=WM(I)/AM1                                                   P1712  00628
   73 CONTINUE                                                         P1712  00629
      FMT(7)=F4                                                        P1712  00630
      WRITE(6,FMT)FMM,FB,FB,FB,(V(J),J=1,NPT)                          P1712  00631
      WRITE(6,FMT)FRA,FR3,FB,FB,(RRHO(J),J=1,NPT)                      P1712  00632
      WRITE(6,FMT)FMA,FMB,FB,FB,(VMOC(J),J=1,NPT)                      P1712  00633
      FMT(7)=F1                                                        P1712  00634
      WRITE(6,FMT) FUD,FL(2),FL(3),FL(4),(SONVEL(J),J=1,NPT)           P1712  00635
      EQL=.TRUE.                                                       P1712  00636
      CALL OUT3                                                        P1712  00637
  865 IF(K.EQ.0) GO TO 1000                                            P1712  00638
      WRITE(6,868)                                                     P1712  00639
  868 FORMAT(1H1)                                                      P1712  00640
      NPT = 0                                                          P1712  00641
  870 NPT = NPT + 1                                                    P1712  00642
C                                                                      P1712  00643
C     SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT                    P1712  00644
C                                                                      P1712  00645
      DO 880 I = 1,NS                                                  P1712  00646
      EN(I,NPT) = EN(I,K)                                              P1712  00647
  880 CONTINUE                                                         P1712  00648
  902 CONTINUE                                                         P1712  00649
 1000 TP = .FALSE.                                                     P1712  00650
      RETURN                                                           P1712  00651
      END                                                              P1712  00652
```

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      C                                                                      P1712   00653
            SUBROUTINE EQLBRM                                                P1712   00654
      C  ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES          P1712   00655
      C                                                                      P1712   00656
      C     DOUBLE PRECISION X,G                                             P1712   00657
            LOGICAL HP,SP,TP,IDEBUG,CONVG,IONS,MOLES,FROZ,EQL,LOGV,HPSP,TPSP P1712   00658
            LOGICAL ISING,IC                                                 P1712   00659
      C                                                                      P1712   00660
            DIMENSION PROW(18)                                               P1712   00661
      C                                                                      P1712   00662
            COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)      P1712   00663
           1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) P1712   00664
           2,TOTN(13)                                                        P1712   00665
            COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150 ,H0(150)  P1712   00666
           1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)            P1712   00667
            COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),BOP(15,2) P1712   00668
           1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712 00669
           2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)        P1712   00670
           3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712 00671
           4 ,RHOP,RMW(15),TLN,JANF                                          P1712   00672
            COMMON /DOUBLE/ G(20,21), X(20)                                  P1712   00673
            COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712 00674
           1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ    P1712   00675
           2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                  P1712   00676
            COMMON/PERF/PCP(26),VMCC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13) P1712 00677
           1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SS0                            P1712   00678
      C                                                                      P1712   00679
            DATA ITER/4HITER/,IE/1HE/,SMALNO/1.E-6/,SMNOL/-13.815511/        P1712   00680
      C                                                                      P1712   00681
            SIZE= 18.5                                                       P1712   00682
            ISING = .FALSE.                                                  P1712   00683
            ENNL = ALOG(ENN)                                                 P1712   00684
            LOGV = .FALSE.                                                   P1712   00685
            PP N = ALOG(PP)                                                  P1712   00686
            TLN = ALOG(TT)                                                   P1712   00687
            CONVG = .FALSE.                                                  P1712   00688
            ITNUMB = ITN                                                     P1712   00689
            IF(IC)  GO TO 966                                                P1712   00690
            IF (.NOT.IONS.OR.IE.EQ.LLMT(L)) GO TO 33                         P1712   00691
            L = L+1                                                          P1712   00692
            IQ1 = IQ1+1                                                      P1712   00693
            DO 499 J = 1,NS                                                  P1712   00694
            IF (A(L,J) .EQ.0.) GO TO 499                                     P1712   00695
            EN(J,NPT) = SMALNO                                               P1712   00696
            ENLN(J) = SMNOL                                                  P1712   00697
            IUSE(J) = 0                                                      P1712   00698
        499 CONTINUE                                                         P1712   00699
         33 IF(NPT.EQ.1 .AND. IDEBUG) WRITE(6,244) (LLMT(I),I=1,L),ITER      P1712   00700
        244 FORMAT (4HOPT ,14(5X,A4))                                        P1712   00701
         43 TM = ALOG(PP/ENN)                                                P1712   00702
            J = 1                                                            P1712   00703
            IF(.NOT.TP) CALL CPHS                                            P1712   00704
            IF(TP.AND.(CONVG.OR.ITNUMB.EQ.ITN)) CALL CPHS                    P1712   00705
```

```
      IF(IC)  GO TO 171                                           P1712  00706
      IF (.NOT.CONVG.OR.JSOL.EQ.0) GO TO 62                       P1712  00707
      ENSOL = EN(JSOL,NPT)                                        P1712  00708
      EN(JSOL,NPT) = EN(JSOL,NPT)+EN(JLIQ,NPT)                    P1712  00709
      IUSE(JLIQ) = -IUSE(JLIQ)                                    P1712  00710
      IQ1 = IQ1-1                                                 P1712  00711
      DLVTP(NPT) = 0.                                             P1712  00712
      CPR(NPT) = 0.                                               P1712  00713
      GAMMAS(NPT) = 0.                                            P1712  00714
      LOGV = .TRUE.                                               P1712  00715
   62 CALL MATRIX                                                 P1712  00716
      NUMB = ITN-ITNUMB+1                                         P1712  00717
      IF(.NOT.CONVG)    GO TO 67                                  P1712  00718
      IF (LOGV.AND.JSOL.EQ.0) GO TO 63                            P1712  00719
      DO 182  I=1,L                                               P1712  00720
      PROW(I) = G(IQ1,I)                                          P1712  00721
  182 CONTINUE                                                    P1712  00722
      IF (.NOT.LOGV) GO TO 67                                     P1712  00723
C                                                                 P1712  00724
C     LOGV = .TRUE.-- SET UP MATRIX TO SOLVE FOR DLVPT            P1712  00725
C                                                                 P1712  00726
   63 G(IQ1,IQ2) = ENN                                            P1712  00727
      IQ = IQ1 - 1                                                P1712  00728
      DO 777 I = 1,IQ                                             P1712  00729
      G(I,IQ2) = G(I,IQ1)                                         P1712  00730
  777 CONTINUE                                                    P1712  00731
   67 IF (.NOT.IDEBUG) GO TO 72                                   P1712  00732
      WRITE(6,772) NUMB                                           P1712  00733
  772 FORMAT (11H0ITERATION  ,I3,6X,7HMATRIX //)                  P1712  00734
      DO 911 I=1,IMAT                                             P1712  00735
  911 WRITE (6,73) (G(I,K),K=1,KMAT)                              P1712  00736
   72 IF(CONVG)  IMAT=IMAT-1                                      P1712  00737
      ITST = IMAT                                                 P1712  00738
      CALL MGAUSD                                                 P1712  00739
      IF(ITST.NE.IMAT)  GO TO 774                                 P1712  00740
      IF(.NOT.IDEBUG.OR.CONVG)  GO TO 773                         P1712  00741
      WRITE (6,373)(LLMT(I),I=1,L)                                P1712  00742
  373 FORMAT (7H0PI     ,9(A4,10X))                               P1712  00743
      WRITE (6,73)(X(I),I=1,IMAT)                                 P1712  00744
   73 FORMAT (9E14.6)                                             P1712  00745
  773 IF(.NOT.CONVG)  GO TO 85                                    P1712  00746
      IF(LOGV)  GO TO 171                                         P1712  00747
  174 SUM = 0.                                                    P1712  00748
      DO 175 J=1,L                                                P1712  00749
      SUM = SUM+PROW(J)*X(J)                                      P1712  00750
  175 CONTINUE                                                    P1712  00751
      DLVTP(NPT) = 1.+G(IQ2,IQ1)/ENN-SUM/ENN  - X(IQ1)            P1712  00752
      CPR(NPT) = G(IQ2,IQ2)                                       P1712  00753
      DO 176 J=1,IQ1                                              P1712  00754
      CPR(NPT) = CPR(NPT)-G(IQ2,J)*X(J)                           P1712  00755
  176 CONTINUE                                                    P1712  00756
      LOGV = .TRUE.                                               P1712  00757
      GO TO 62                                                    P1712  00758
```

```
      C
      C  SINGULAR MATRIX
      C
        774 IF(.NOT.CONVG)  GO TO 775
            WRITE(6,172)
        172 FORMAT(25H0DERIVATIVE MATRIX SINGULAR )
            IC = .TRUE.
            GO TO 171
        775 IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 371
            WRITE(6,874)
        874 FORMAT(96H0LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE
           1BEEN INCLUDED ON AN INSERT CARD, RESTART )
            GO TO 873
        871 WRITE (6,74)
         74 FORMAT(16H0SINGULAR MATRIX)
            IF(IC)  GO TO 873
            IF (ISING) GO TO 937
            NTZERO = 0
        965 DO 970 JJ = 1, NS
            IF(IUSE(JJ)) 970,968,967
        967 IF(EN(JJ,NPT).EQ.0.)  GO TO 873
            GO TO 969
        968 IF(EN(JJ,NPT).NE.0.)  GO TO 969
            EN(JJ,NPT) = SMALNO
            ENLN(JJ) = SMNOL
            GO TO 970
        969 NTZERO = NTZERO+1
        970 CONTINUE
            IF(.NOT.IC)  GO TO 971
            IC = .FALSE.
            GO TO 43
        971 ISING = .TRUE.
            WRITE (6,776)
        776 FORMAT (8H0RESTART)
            GO TO 43
        997 IF(NTZERO.NE.(L-1))  GO TO 873
            IF(EQRAT.GT.1.00001.OR.EQRAT.LT.0.99999) GO TO 873
            ENN=0.
            NEN = 0
            DO 83  I=1,L
            JEN=0
            DO 80  J=1,NS
            IF(EN(J,NPT).EQ.0.)  GO TO 80
            IF(A(I,J).EQ.0.)  GO TO 83
            IF(JEN.NE.0)  GO TO 83
            JEN = J
         80 CONTINUE
            NEN = NEN+1
            EN(JEN,NPT) = B0(I)/A(I,JEN)
         83 CONTINUE
            IF(NEN.LT.NTZERO)  GO TO 373
            CONVG = .TRUE.
            IC = .TRUE.
```

```
      HSUM(NPT) = 0.
      DO 84  J=1,NS
      IF(EN(J,NPT).EQ.0.)  GO TO 84
      ENN = EN(J,NPT)+ENN
      TEM = EN(J,NPT)
      ENLN(J) = ALOG(TEM)
      HSUM(NPT) = HSUM(NPT) + EN(J,NPT)*H0(J)
   84 CONTINUE
      TM = ALOG(PP/ENN)
      GO TO 43
   85 ITNUMB= ITNUMB-1
C
C     OBTAIN CORRECTIONS TO THE ESTIMATES
C
      KK = L + 1
      DLNT= X(IQ2)
      IF (TP) DLNT=0.
      DO 101 J=1,NS
      IF (IUSE(J)) 101,98,100
   98 DELN(J) = H0(J)*DLNT-H0(J)+S(J)-ENLN(J)-TM+X(IQ1)
      DO 99 K=1,L
      DELN(J)= DELN(J)+A(K,J)*X(K)
   99 CONTINUE
      GO TO 101
  100 DELN(J) = X(KK)
      KK = KK + 1
  101 CONTINUE
      AMBDA= 1.
      AMBDA1= 1.
      SUM = X(IQ1)
      IF(SUM.LT.0.)  SUM=-SUM
      IF(DLNT.GT.SUM)  SUM=DLNT
      IF(-DLNT.GT.SUM)  SUM=-DLNT
      DO 917 J=1,NS
      IF (IUSE(J).NE.0) GO TO 917
      IF((EN(J,NPT).GT.0.).AND.DELN(J).GT.SUM)  SUM = DELN(J)
      IF((EN(J,NPT).NE.0.) .OR. DELN(J).LE.0.) GO TO 917
      SUM1 = (-9.212-ENLN(J)+ENNL)/(DELN(J)-X(IQ1))
      IF(SUM1.LT.0.)  SUM1=-SUM1
      IF (SUM1.LT.AMBDA1) AMBDA1 = SUM1
  917 CONTINUE
      IF(SUM.GT.2.)AMBDA=2./SUM
      IF (AMBDA1.LT.AMBDA) AMBDA = AMBDA1
      IF (.NOT.IDEBUG) GO TO 111
      WRITE(6,923) TT,ENN,ENNL,PP,PPLN,AMBDA
  923 FORMAT (3H0T=,E15.8,6H  ENN=,E15.8,7H  ENNL=E15.8,5H  PP=,E15.8,
     1 7H  PPLN=E15.8,8H  AMBDA=E15.8 )
      WRITE (6,924)
  924 FORMAT(1H0,18X,2HNI,12X,5HLN NI,8X,9HDEL LN NI,10X,4HH/RT,9X,4HS0/
     1R,12X,6H-G0/RT,9X,5H-G/RT  )
      DO 926 J=1,NS
      FNEG1 = S(J)-H0(J)
      FNEG2 = FNEG1
```

```
      IF(IUSE(J).EQ.0)  FNEG2=FNEG2-ENLN(J)-TM
      WRITE (6,925) SUB(J,1),SUB(J,2),
     1SUB(J,3),EN(J,NPT),ENLN(J),DELN(J),H0(J),S(J),FNEG1,FNEG2
  925 FORMAT (1X,3A4,7E15.6)
  926 CONTINUE
      WRITE (6,110)
  110 FORMAT(1H0)
C
C     APPLY CORRECTIONS TO ESTIMATES
C
  111 SUM = 0.
      DO 113 J=1,NS
      IF (IUSE(J)) 113,112,114
  112 ENLN(J)=ENLN(J)+AMBDA*DELN(J)
      EN(J,NPT) = 0.
      IF((ENLN(J)-ENNL+SIZE).LE.0.)  GO TO 113
      EN(J,NPT) = EXP(ENLN(J))
      SUM = SUM+EN(J,NPT)
      GO TO 113
  114 EN(J,NPT) = EN(J,NPT) + AMBDA * DELN(J)
  113 CONTINUE
      SUMN = SUM
      IF (TP) GO TO 115
      TLN= TLN+AMBDA*DLNT
      TT     = EXP(TLN)
  115 ENNL = ENNL+AMBDA*X(IG1)
      ENN = EXP(ENNL)
      IF (LLMT(L).NE.IE) GO TO 116
C
C     CHECK ON REMOVING IONS
C
      DO 1116 J = 1,NS
      IF (A(L,J).EQ.0.) GO TO 1116
      IF (EN(J,NPT).GT.0.) GO TO 116
 1116 CONTINUE
      DO 1118  J=1,NS
      IF(A(L,J).NE.0.) IUSE(J) = -10000
 1118 CONTINUE
      L = L-1
      IG1 = IG1-1
      GO TO 43
C
C     TEST FOR CONVERGENCE
C
  116 IF (ITNUMB.EQ.0) GO TO 13
      IF (AMBDA.LT.1.) GO TO 43
      SUM = (ENN-SUMN)/ENN
      IF (SUM.LT.0.) SUM = -SUM
      IF (SUM.GT.0.5E-5) GO TO 43
      DO 130 J=1,NS
      IF (IUSE(J).LT.0) GO TO 130
      AA= DELN(J)/SUMN
      IF(AA.LT.0.)  AA=-AA
```

```
      IF (IUSE(J).EQ.0) AA = AA+EN(J,NPT)                                P1712  00918
  129 IF(AA.GT.0.5E-5)  GO TO 43                                         P1712  00919
  130 CONTINUE                                                           P1712  00920
   13 CONVG= .TRUE.                                                      P1712  00921
      IF(TT.LT.TLOW.OR.TT.GT.THIGH.AND.IDEBUG) WRITE(6,306) TT,NPT       P1712  00922
  306 FORMAT(17H0THE TEMPERATURE=E12.4,26H IS OUT OF RANGE FOR POINT,I5) P1712  00923
      IF(ITNUM3.NE.3) GO TO 165                                          P1712  00924
      WRITE(6,973) ITN,NPT                                               P1712  00925
  973 FORMAT(1H0,I2,69H ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREME P1712  00926
     1NTS FOR THE POINT        I5)                                       P1712  00927
      IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 873       P1712  00928
      WRITE(6,874)                                                       P1712  00929
      TT = T(1)                                                          P1712  00930
      RETURN                                                             P1712  00931
C                                                                        P1712  00932
C     CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES.           P1712  00933
C                                                                        P1712  00934
  160 IF(NC.EQ.0) GO TO 143                                              P1712  00935
      SIZEF = 0.                                                         P1712  00936
      INC = 0                                                            P1712  00937
      DO 170 J = 1,NS                                                    P1712  00938
      IF (IUSE(J).EQ.0 .OR. IUSE(J).EQ.-10000) GO TO 170                 P1712  00939
      INC = INC + 1                                                      P1712  00940
      IF(IDEBUG) WRITE(6,144)(SUB(J,I),I=1,3),TEMP(INC,1),TEMP(INC,2),   P1712  00941
     1IUSE(J),EN(J,NPT)                                                  P1712  00942
  144 FORMAT (1H0,3A4,2F10.3,3X,6HIUSE=,I4,E15.7)                        P1712  00943
      IF (EN(J,NPT)) 146,148,159                                         P1712  00944
  146 IF (J.NE.JSOL .AND. J .NE.JLIQ) GO TO 147                          P1712  00945
      JSOL = 0                                                           P1712  00946
      JLIQ = 0                                                           P1712  00947
  147 IGI = IGI - 1                                                      P1712  00948
      EN(J,NPT) = 0.                                                     P1712  00949
      GO TO 166                                                          P1712  00950
  148 KG = 1                                                             P1712  00951
      IF(IUSE(J).EQ.-IUSE(J+1)) GO TO 154                                P1712  00952
  151 IF(J.EQ.1.OR.IUSE(J).NE.-IUSE(J-1)) GO TO 153                      P1712  00953
      KG = -1                                                            P1712  00954
  154 JKG = J + KG                                                       P1712  00955
      IF (EN(JKG,NPT).LT.0.) GO TO 170                                   P1712  00956
      TMELT = TEMP(INC,1)                                                P1712  00957
      IMP = INC + KG                                                     P1712  00958
      IF(TMELT.EQ.TEMP(IMP,2  )) GO TO 158                               P1712  00959
      TMELT = TEMP(INC,2)                                                P1712  00960
      IF (TMELT.EQ.TEMP(IMP,1)) GO TO 157                                P1712  00961
      WRITE (6,156)                                                      P1712  00962
  156 FORMAT (50H03 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER  )    P1712  00963
C                                                                        P1712  00964
C  JTH SPECIES A SOLID (EN=0), (J+KG)TH SPECIES A LIQUID (EN IS +)       P1712  00965
C                                                                        P1712  00966
  157 IF(TT.GT.TMELT) GO TO 169                                          P1712  00967
      IF (TP.AND.TT.EQ.TMELT) GO TO 169                                  P1712  00968
      IF (TP)  GO TO 1165                                                P1712  00969
      IF (TT.LE.TMELT-150.) GO TO 1165                                   P1712  00970
```

```
      JSOL = J                                                         P1712 00971
      JLIQ = JKG                                                       P1712 00972
      GO TO 159                                                        P1712 00973
C                                                                      P1712 00974
C  JTH SPECIES A LIQUID(EN=0), (J+KG)TH SPECIES A SOLID (EN IS +)      P1712 00975
C                                                                      P1712 00976
  158 IF (TT.LT.TMELT) GO TO 169                                       P1712 00977
      IF (TP.AND.TT.EQ.TMELT) GO TO 169                                P1712 00978
      IF (TP)   GO TO 1165                                             P1712 00979
      IF (TT.GE.TMELT+150.) GO TO 1165                                 P1712 00980
      JSOL = JKG                                                       P1712 00981
      JLIQ = J                                                         P1712 00982
  159 TLN = ALOG (TMELT)                                               P1712 00983
      TT = TMELT                                                       P1712 00984
      EN(JKG,NPT) = .5 * EN(JKG,NPT)                                   P1712 00985
      EN(J,NPT) = EN(JKG,NPT)                                          P1712 00986
      GC TO 165                                                        P1712 00987
C                                                                      P1712 00988
C  WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH EN                      P1712 00989
C                                                                      P1712 00990
 1165 EN(J,NPT) = EN (JKG, NPT)                                        P1712 00991
      IUSE(J) = -IUSE(J)                                               P1712 00992
      IUSE (JKG) = -IUSE(JKG)                                          P1712 00993
      EN(JKG,NPT)= 0.                                                  P1712 00994
      GO TO 40                                                         P1712 00995
  153 IF (TT.LT.TEMP(INC,1) .AND.TEMP(INC,1).NE.TLOW) GO TO 169        P1712 00996
      IF (TT.GT.TEMP(INC,2)) GO TO 169                                 P1712 00997
C                                                                      P1712 00998
C                                                                      P1712 00999
      SUM = 0.                                                         P1712 01000
      DO 167 I = 1,L                                                   P1712 01001
      SUM = SUM + A(I,J)*X(I)                                          P1712 01002
  167 CONTINUE                                                         P1712 01003
      DELF = H0(J)-S(J)-SUM                                            P1712 01004
      IF(IDEBUG) WRITE(6,168)DELF,SIZEF                                P1712 01005
  168 FORMAT (17H G0-SUM(AIJ*PI) =E15.7,10X,18HPREVIOUS DELTA G =,E15.7) P1712 01006
      IF(DELF.GE.SIZEF .OR. DELF.GE.0.) GO TO 169                      P1712 01007
      SIZEF = DELF                                                     P1712 01008
      JDELF = J                                                        P1712 01009
  169 IF(INC.EQ.NC) GO TO 1160                                         P1712 01010
  170 CONTINUE                                                         P1712 01011
 1160 IF (SIZEF.EQ.0.) GO TO 143                                       P1712 01012
      J = JDELF                                                        P1712 01013
  165 IC1 = IC1 + 1                                                    P1712 01014
  166 IUSE(J) = - IUSE(J)                                              P1712 01015
   40 CONVG = .FALSE.                                                  P1712 01016
  143 TN = NUMB                                                        P1712 01017
      IF(IDEBUG) WRITE(6,771) NPT, (X(IL),IL=1,L), TN                  P1712 01018
  771 FORMAT (I3,14F9.3)                                               P1712 01019
      ITNUMB = ITN                                                     P1712 01020
      GO TO 43                                                         P1712 01021
C                                                                      P1712 01022
C     CALCULATE EQUILIBRIUM PROPERTIES                                 P1712 01023
```

```
C
  171 SSUM(NPT) = 0.
      IF(JLIQ.NE.0) EN(JSOL,NPT)=ENSOL
      DO 183 J=1,NS
      IF (NPT.EQ.1) SS0 = SS0 + EN(J,1)*S(J)
      SS = S(J)
      IF(IUSE(J).EQ.0)  SS=SS-ENLN(J)-T4
      SSUM(NPT) = SSUM(NPT)+SS*EN(J,NPT)
  183 CONTINUE
      IF(.NOT.IC)  GO TO 176
      DLVPT(NPT) = -1.
      DLVTP(NPT) = 1.
      CPR(NPT) = CPSUM
      GO TO 199
  176 SUM = 0.
      DO 179 J = 1,L
      SUM = SUM + PROR(J)*X(J)
  179 CONTINUE
      DLVPT(NPT) = -2.+SUM/ENN+ X(IQ1)
  184 IF(JLIQ.EQ.0)  GO TO 199
      IUSE(JLIQ) = -IUSE(JLIQ)
      HSUM(NPT) = HSUM(NPT)+EN(JLIQ,NPT)*(H0(JLIQ)-H0(JSOL))
      IQ1 = IQ1+1
      GAMMAS(NPT) = -1./DLVPT(NPT)
      GO TO 186
  199 GAMMAS(NPT) = -1./(DLVPT(NPT)+(DLVTP(NPT)**2)*ENN/CPR(NPT))
  186 TTT(NPT) = TT
      PPP(NPT) = PP
      CPRF(NPT) = CPSUM
      HSUM(NPT) = HSUM(NPT)*TT
      WM(NPT) = 1./ENN
  200 IF (.NOT.IDEBUG) RETURN
      WRITE(6,201) NPT,PCP(NPT),PP,TT,HSUM(NPT),SSUM(NPT),WM(NPT),CPR(NP
     1T),DLVPT(NPT),DLVTP(NPT),GAMMAS(NPT)
  201 FORMAT (7H0POINT=I3,3X,4HPCP=E13.6,3X,2HP=E13.6,3X,2HT=E13.6,3X,4H
     1H/R=E13.6,3X,4HS/R=E13.6//3X,3HMW=E13.6,3X,5HCP/R=E13.6,3X,6HDLVPT
     2=E13.6,3X,6HDLVTP=E13.6,3X,9HGAMMA(S)=E13.6 )
      GO TO 1000
C
C     ERROR, SET TT=0
C
  873 TT=0.
      NPT = NPT-1
 1000 RETURN
      END
```

```
      SUBROUTINE FROZEN                                                 P1712 01069
C                                                                       P1712 01070
C                                                                       P1712 01071
C     (FROZEN COMPOSITION EXPANSION ONLY)                               P1712 01072
C                                                                       P1712 01073
      LOGICAL EQL,FROZ,CONVG                                            P1712 01074
C                                                                       P1712 01075
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)       P1712 01076
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)  P1712 01077
     2,TCTN(13)                                                         P1712 01078
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)   P1712 01079
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)             P1712 01080
      COMMON/MISC/ENN,SUMN,TT,SM,ATOM(3,101),ILMT(15),BO(15),BOP(15,2)  P1712 01081
     1 ,TM,TLOW,TMID,THIGH,PCSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AC(2),AM(2)   P1712 01082
     2 ,HPP(2),RHO(2),VMIN(2),ALS(2),WP(2),DATA(22),NAME(15,5)          P1712 01083
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712 01084
     4 ,RHOP,RMW(15),TLN,JANF                                           P1712 01085
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712 01086
     1 KMAT,IMAT,IQI,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ      P1712 01087
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                   P1712 01088
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13) P1712 01089
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSO                             P1712 01090
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)     P1712 01091
     1   ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2       P1712 01092
     2   ,FRI,FCI,FN(4),FR(4),FA(4),FI(4),FMT9X,FO                      P1712 01093
      ITROT = 3                                                         P1712 01094
      EQL =.FALSE.                                                      P1712 01095
      NPT = 2                                                           P1712 01096
       TT = TTT(1)                                                      P1712 01097
      TLN=ALOG(TT)                                                      P1712 01098
      GAMMAS(1) = CPRF(1)/(CPRF(1)-1./WM(1))                            P1712 01099
      CPR(1) = CPRF(1)                                                  P1712 01100
      PCP(2) = ((GAMMAS(1)+1.)/2.)**(GAMMAS(1)/(GAMMAS(1)-1.))          P1712 01101
      DATA(1) = 2./(GAMMAS(1) + 1.)                                     P1712 01102
      TLN = TLN + ALOG(DATA(1))                                         P1712 01103
      DO 902  IP=2,NP                                                   P1712 01104
      IF(NPT.EQ.2)  GO TO 45                                            P1712 01105
      PCP(NPT) = P(1)/P(IP)                                             P1712 01106
   45 CONVG = .FALSE.                                                   P1712 01107
      PCPLN= ALOG(PCP(NPT))                                             P1712 01108
      SO = SSO -PCPLN/WM(1)                                             P1712 01109
      SUMH = 0.                                                         P1712 01110
   51 TT=EXP(TLN)                                                       P1712 01111
      SUMS=0.                                                           P1712 01112
      J = 1                                                             P1712 01113
      NNN = NPT                                                         P1712 01114
      NPT = 1                                                           P1712 01115
      CALL CPHS                                                         P1712 01116
      NPT = NNN                                                         P1712 01117
      DO 60 J=1,NS                                                      P1712 01118
      IF(EN(J,1).EQ.0.)  GO TO 60                                       P1712 01119
      SUMS = SUMS + S(J)*EN(J,1)                                        P1712 01120
      IF(CONVG) SUMH=SUMH+HO(J)*EN(J,1)                                 P1712 01121
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   69 CONTINUE                                                         P1712   01122
      IF (CONVG) GO TC 81                                              P1712   01123
      DLNT=(SUMS-S0)/CPSUM                                             P1712   01124
      TLN=TLN-DLNT                                                     P1712   01125
      IF(DLNT.LT.0.) DLNT=-DLNT                                        P1712   01126
      IF(DLNT.LT.0.5E-4)  CONVG=.TRUE.                                 P1712   01127
      GO TO 51                                                         P1712   01128
   81 TTT(NPT)= TT                                                     P1712   01129
      SSUM(NPT)= SSUM(1)                                               P1712   01130
      HSUM(NPT)= TT*SUMH                                               P1712   01131
      GAMMAS(NPT)= CPSUM/(CPSUM-1./WM(1))                              P1712   01132
      IF(IP.GT.2)  GO TO 90                                            P1712   01133
C                                                                      P1712   01134
C     THROAT CALCULATIONS                                              P1712   01135
C                                                                      P1712   01136
      DH = HSUM(1)-HSUM(2)                                             P1712   01137
      DHSTAR = DH-(GAMMAS(2)*TT/(2.*WM(1)))                            P1712   01138
      DH = DHSTAR/DH                                                   P1712   01139
      IF(DH.LT.0.)  DH=-DH                                             P1712   01140
      IF(DH.LT 0.4E-4.OR.ITROT.EQ.0) GO TO 90                          P1712   01141
      PCP(2) = PCP(2)/(1.+2.*DHSTAR*WM(1)/(TT*(GAMMAS(2)+1.)))         P1712   01142
      P(2) = P(1)/PCP(2)                                               P1712   01143
      ITROT = ITROT-1                                                  P1712   01144
      GO TO 45                                                         P1712   01145
   90 WP(NPT)= WM(1)                                                   P1712   01146
      PPP(NPT) = P(IP)                                                 P1712   01147
      CPR(NPT)= CPSUM                                                  P1712   01148
      K = 0                                                            P1712   01149
      IF (TT.LT.(TLOW-150.))GO TO 903                                  P1712   01150
      IF(NC.EQ.0) GO TO 700                                            P1712   01151
      INC = 0                                                          P1712   01152
      DO 901 I=1,NS                                                    P1712   01153
      IF(IUSE(I).EQ.0.OR.IUSE(I).EQ.-10000) GO TO 901                  P1712   01154
      INC = INC+1                                                      P1712   01155
      IF(EN(I,1).EQ.0.) GO TO 901                                      P1712   01156
      IF (TT.LT.(TEMP(INC,1)-50.).OR.TT.GT.(TEMP(INC,2)+50.))GO TO 903 P1712   01157
  901 CONTINUE                                                         P1712   01158
  700 IF ( IP.EQ.NP) GO TO 863                                         P1712   01159
      K = NPT                                                          P1712   01160
      IF (NPT.NE.13) GO TO 870                                         P1712   01161
      GO TO 863                                                        P1712   01162
  903 NPT = NPT - 1                                                    P1712   01163
  863 CALL RKTOUT                                                      P1712   01164
      IF (NSUB+NSUP.NE.0) CALL RATIO                                   P1712   01165
  865 IF (K.EQ.0) GO TO 1000                                           P1712   01166
      NPT = 2                                                          P1712   01167
  870 NPT = NPT + 1                                                    P1712   01168
  902 CONTINUE                                                         P1712   01169
 1000 RETURN                                                           P1712   01170
      END                                                              P1712   01171
```

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      C                                                                      P1712   01172
            SUBROUTINE HCALC                                                 P1712   01173
      C                                                                      P1712   01174
      C  CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS                 P1712   01175
      C                                                                      P1712   01176
            LOGICAL MOLES                                                    P1712   01177
            DIMENSION NUM(15,5),WS(2)                                        P1712   01178
      C                                                                      P1712   01179
            COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)  P1712   01180
           1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)            P1712   01181
            COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),3U(15),B0P(15,2) P1712   01182
           1 ,TM,TLOW,THID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712   01183
           2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)        P1712   01184
           3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712   01185
           4 ,RHOP,RMW(15),TLN,JANF                                          P1712   01186
            COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712   01187
           1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ    P1712   01188
           2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                  P1712   01189
      C                                                                      P1712   01190
            EQUIVALENCE(ANUM,NUM)                                            P1712   01191
      C                                                                      P1712   01192
            DATA AG/1HG/,IZERO/2H00/,OX/1HO/                                 P1712   01193
      C                                                                      P1712   01194
      C  IS TT IN RANGE                                                      P1712   01195
      C                                                                      P1712   01196
            IF(TT.LT.(TLOW-100.).OR.TT.GT.(THIGH+1000.))GO TO 80             P1712   01197
            WS(1) = 0.                                                       P1712   01198
            WS(2) = 0.                                                       P1712   01199
            HPP(1)=0.                                                        P1712   01200
            HPP(2)=0.                                                        P1712   01201
            AC(1)=0.                                                         P1712   01202
            AC(2)=0.                                                         P1712   01203
            DO 900 N=1,NREAC                                                 P1712   01204
            K=2                                                              P1712   01205
            IF(FOX(N).EQ.OX)K=1                                              P1712   01206
            PCWT=PECWT(N)                                                    P1712   01207
            IF(MOLES)PCWT=PCWT*RMW(N)                                        P1712   01208
            WS(K) = WS(K) + PCWT                                             P1712   01209
            J = NUM(N,5)                                                     P1712   01210
            IF (J.NE.0) GO TO 90                                             P1712   01211
            DO 10 J=1,L                                                      P1712   01212
            DATA(J)=0.                                                       P1712   01213
         10 CONTINUE                                                         P1712   01214
            DO 40 I=1,4                                                      P1712   01215
            IF(ANUM(N,I).EQ.0.)GO TO 50                                      P1712   01216
            DO 20 J=1,L                                                      P1712   01217
            IF(LLMT(J).EQ.NAME(N,I))  GO TO 30                               P1712   01218
         20 CONTINUE                                                         P1712   01219
         30 DATA(J)=ANUM(N,I)                                                P1712   01220
         40 CONTINUE                                                         P1712   01221
         50 IS=0                                                             P1712   01222
            DO 70 J=1,NS                                                     P1712   01223
            IF(IUSE(J).EQ.0)GO TO 55                                         P1712   01224
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```
      IS = IS+1                                                  P1712   01225
      IF(FAZ(N).EQ.AG)GO TO 70                                   P1712   01226
      IF(TT.LT.TEMP(IS,1).OR.TT.GT.TEMP(IS,2)) GO TO 70          P1712   01227
      GO TO 56                                                   P1712   01228
   55 IF(FAZ(N).NE.AG) GO TO 70                                  P1712   01229
   56 DO 60 I=1,L                                                P1712   01230
      IF(A(I,J).NE.DATA(I))  GO TO 70                            P1712   01231
   60 CONTINUE                                                   P1712   01232
      NUM(N,5) = J                                               P1712   01233
      GO TO 90                                                   P1712   01234
   70 CONTINUE                                                   P1712   01235
      GO TO 80                                                   P1712   01236
   90 NSS = NS                                                   P1712   01237
      NS = J                                                     P1712   01238
      CALL CPHS                                                  P1712   01239
      CPSUM = CPSUM/EN(J,NPT)                                    P1712   01240
      NS = NSS                                                   P1712   01241
      IF (HO(J).GT.-.01 .AND. HO(J).LT..01) HO(J) = 0.           P1712   01242
      RTEMP(N) = TT                                              P1712   01243
      ENTH(N) = HO(J)*R*TT                                       P1712   01244
      AC(K)=AC(K)+CPSUM*PCWT/RMW(N)                              P1712   01245
  500 HPP(K)=HPP(K)+ENTH(N)*PCWT/RMW(N)                          P1712   01246
  900 CONTINUE                                                   P1712   01247
      DO 950 K=1,2                                               P1712   01248
      IF(WP(K).EQ.0.)GO TO 950                                   P1712   01249
      HPP(K)=HPP(K)/WS(K)                                        P1712   01250
      AC(K)=AC(K)/WS(K)                                          P1712   01251
  950 CONTINUE                                                   P1712   01252
      HSUBO = (WP(1)*HPP(1)+WP(2)*HPP(2))/(WP(1)+WP(2))          P1712   01253
      GO TO 1000                                                 P1712   01254
   80 WRITE(6,85) N                                              P1712   01255
   85 FORMAT(1H0,I2,34HITH REACTANT IS NOT IN THERMO DATA )      P1712   01256
 1000 RETURN                                                     P1712   01257
      END                                                        P1712   01258
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      SUBROUTINE MATRIX                                                 P1712   01259
C                                                                       P1712   01260
C                                                                       P1712   01261
C     DOUBLE PRECISION G,X                                              P1712   01262
      LOGICAL HP,SP,TF,IDEBUG,CONVG,NEWR                                P1712   01263
C                                                                       P1712   01264
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)      P1712   01265
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) P1712   01266
     2,TCTN(13)                                                         P1712   01267
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)  P1712   01268
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)            P1712   01269
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),BOP(15,2) P1712   01270
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712 01271
     2 ,PPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)        P1712   01272
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712 01273
     4 ,RHOP,RMW(15),TLN,JANF                                           P1712   01274
      COMMON /DOUBLE/ G(20,21), X(20)                                   P1712   01275
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  01276
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ     P1712   01277
     2 ,IONS,AC,NSERT,JSOL,JLIO,KASE(14),NREAC,IC,IQ2                   P1712   01278
C                                                                       P1712   01279
      IQ2 = IQ1 + 1                                                     P1712   01280
      IQ3 = IQ2 + 1                                                     P1712   01281
      KMAT = IQ3                                                        P1712   01282
      IF(.NOT.CONVG.AND.TP) KMAT = IQ2                                  P1712   01283
      IMAT = KMAT - 1                                                   P1712   01284
C                                                                       P1712   01285
C     CLEAR MATRIX STORAGES TO ZERO                                     P1712   01286
C                                                                       P1712   01287
      DO 211 I=1,IMAT                                                   P1712   01288
      DO 211 K=1,KMAT                                                   P1712   01289
C     G(I,K)= 0.0D0                                                     P1712   01290
      G(I,K)= 0.0                                                       P1712   01291
  211 CONTINUE                                                          P1712   01292
      SSS = 0.                                                          P1712   01293
      HSUM(NPT) = 0.                                                    P1712   01294
C                                                                       P1712   01295
C     BEGIN SET UP OF ITERATION MATRIX                                  P1712   01296
C                                                                       P1712   01297
      KK = L                                                            P1712   01298
      DO 65  J=1,NS                                                     P1712   01299
      H=H0(J)*EN(J,NPT)                                                 P1712   01300
      IF (IUSE(J)) 65,11,70                                             P1712   01301
   11 F = (H0(J)-S(J)+ENLN(J)+TM)*EN(J,NPT)                             P1712   01302
      SS = H-F                                                          P1712   01303
      TERM1 = H                                                         P1712   01304
      IF (KMAT .EQ. IQ2) TERM1 = F                                      P1712   01305
      DO 55 I = 1, L                                                    P1712   01306
C                                                                       P1712   01307
C     CALCULATE THE ELEMENTS  R(I,K)                                    P1712   01308
C                                                                       P1712   01309
      IF (A(I,J) .EQ. 0.) GO TO 55                                      P1712   01310
      TERM= A(I,J)*EN(J,NPT)                                            P1712   01311
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            DO 15  K=I,L                                          P1712  01312
            G(I,K)= G(I,K) + A(K,J)*TERM                          P1712  01313
         15 CONTINUE                                              P1712  01314
      C                                                           P1712  01315
            G(I,IQ1)=G(I,IQ1)+TERM                                P1712  01316
            G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM1                        P1712  01317
            IF (CONVG .OR.TP) GO TO 55                            P1712  01318
            G(I,IQ3)= G(I,IQ3)+A(I,J)*F                           P1712  01319
            IF (SP) G(IQ2,I) = G(IQ2,I) + A(I,J)*SS               P1712  01320
         55 CONTINUE                                              P1712  01321
            IF (KMAT .EQ. IQ2) GO TO 64                           P1712  01322
            IF(CONVG.OR.HP) GO TO 59                              P1712  01323
            G(IQ2,IQ1) = G(IQ2,IQ1) + SS                          P1712  01324
            G(IQ2,IQ2)=G(IQ2,IQ2)+H0(J)*SS                        P1712  01325
            G(IQ2,IQ3) = G(IQ2,IQ3)+(S(J) - ENLN(J)-TM)*F         P1712  01326
            GO TO 62                                              P1712  01327
         59 G(IQ2,IQ2)=G(IQ2,IQ2)+H0(J)*H                         P1712  01328
            IF (CONVG) GO TO 64                                   P1712  01329
            G(IQ2,IQ3)=G(IQ2,IQ3)+H0(J)*F                         P1712  01330
         62 G(IQ1,IQ3)=G(IQ1,IQ3)+F                               P1712  01331
         64 G(IQ1,IQ2)=G(IQ1,IQ2)+TERM                            P1712  01332
            GO TO 65                                              P1712  01333
      C                                                           P1712  01334
      C   CONDENSED SPECIES                                       P1712  01335
      C                                                           P1712  01336
         70 KK = KK + 1                                           P1712  01337
            DO 75  I = 1,L                                        P1712  01338
            G(I,KK) = A(I,J)                                      P1712  01339
            G(I,KMAT) = G(I,KMAT) - A(I,J)*EN(J,NPT)              P1712  01340
         75 CONTINUE                                              P1712  01341
            G(KK,IQ2) = H0(J)                                     P1712  01342
            G(KK,KMAT) = H0(J) - S(J)                             P1712  01343
            HSUM(NPT) = HSUM(NPT)+ H                              P1712  01344
            IF(.NOT.SP) GO TO 65                                  P1712  01345
            SSS = SSS + S(J)*EN(J,NPT)                            P1712  01346
            G(IQ2,KK) = S(J)                                      P1712  01347
         65 CONTINUE                                              P1712  01348
            SSS = SSS + G(IQ2,IQ1)                                P1712  01349
            HSUM(NPT) = HSUM(NPT) + G(IQ1,IQ2)                    P1712  01350
            G(IQ1,IQ1) = SUMN - ENN                               P1712  01351
      C                                                           P1712  01352
      C     REFLECT SYMMETRIC PORTIONS OF THE MATRIX              P1712  01353
      C                                                           P1712  01354
            ISYM = IQ1                                            P1712  01355
            IF(HP.OR.CONVG)ISYM=IQ2                               P1712  01356
            DO 102 I=1,ISYM                                       P1712  01357
            DO 102 J=I,ISYM                                       P1712  01358
            G(J,I)=G(I,J)                                         P1712  01359
        102 CONTINUE                                              P1712  01360
      C                                                           P1712  01361
      C     COMPLETE THE RIGHT HAND SIDE                          P1712  01362
      C                                                           P1712  01363
            IF(CONVG)  GO TO 175                                  P1712  01364
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          DO 145 I=1,L                                       P1712   01365
          X(1)=B0(I)-G(I,IQ1)                                P1712   01366
          G(I,KMAT) = G(I,KMAT)+X(1)                         P1712   01367
      145 CONTINUE                                           P1712   01368
          G(IQ1,KMAT) = G(IQ1,KMAT)+ENN-SUMN                 P1712   01369
C                                                            P1712   01370
C         COMPLETE ENERGY ROW AND TEMPERATURE COLUMN         P1712   01371
C                                                            P1712   01372
          IF (KMAT .EQ. IQ2) GO TO 185                       P1712   01373
          IF (SP)ENERGY = S0+ENN-SUMN - SSS                  P1712   01374
          IF(HP)ENERGY=HSUB0/TT - HSUM(NPT)                  P1712   01375
          G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY                      P1712   01376
      175 G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM                       P1712   01377
      185 RETURN                                             P1712   01378
          END                                                P1712   01379
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      SUBROUTINE MGAUSD                                              P1712  01380
C                                                                    P1712  01381
C     SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS                     P1712  01382
C                                                                    P1712  01383
C     DOUBLE PRECISION G,X,COEFX(20),SUM,Z                           P1712  01384
      DIMENSION COEFX(20)                                            P1712  01385
C                                                                    P1712  01386
      COMMON/DOUBLE/G(20,21),X(20)                                   P1712  01387
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  01388
     1 KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ   P1712  01389
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                P1712  01390
C                                                                    P1712  01391
      EQUIVALENCE (IUSE,IMAT)                                        P1712  01392
C                                                                    P1712  01393
      DATA BIGNO/1.E+38/                                             P1712  01394
C                                                                    P1712  01395
C     BEGIN ELIMINATION OF NNTH VARIABLE                             P1712  01396
C                                                                    P1712  01397
      IUSE1=IUSE+1                                                   P1712  01398
    6 DO 45 NN=1,IUSE                                                P1712  01399
      IF (NN-IUSE) 8,83,8                                            P1712  01400
   83 IF(G(NN,NN))31,23,31                                           P1712  01401
C                                                                    P1712  01402
C     SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW                     P1712  01403
C                                                                    P1712  01404
    8 DO 18 I=NN,IUSE                                                P1712  01405
      COEFX(I) = BIGNO                                               P1712  01406
      IF(G(I,NN).EQ.0.)  GO TO 18                                    P1712  01407
      COEFX(I) = 0.                                                  P1712  01408
      DO 10 J=NN,IUSE1                                               P1712  01409
      SUM = G(I,J)                                                   P1712  01410
      IF(SUM.LT.0.)  SUM=-SUM                                        P1712  01411
      IF(J.NE.NN)  GO TO 9                                           P1712  01412
      Z = SUM                                                        P1712  01413
      GO TO 10                                                       P1712  01414
    9 IF(SUM.GT.COEFX(I))  COEFX(I)=SUM                              P1712  01415
   10 CONTINUE                                                       P1712  01416
      COEFX(I) = COEFX(I)/Z                                          P1712  01417
   18 CONTINUE                                                       P1712  01418
      TEMP = BIGNO                                                   P1712  01419
      I=0                                                            P1712  01420
   20 DO 22 J=NN,IUSE                                                P1712  01421
      IF (COEFX(J)-TEMP) 87,22,22                                    P1712  01422
   87 TEMP=COEFX(J)                                                  P1712  01423
      I=J                                                            P1712  01424
   22 CONTINUE                                                       P1712  01425
      IF(I) 28,23,28                                                 P1712  01426
C                                                                    P1712  01427
C     INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH    P1712  01428
C     VARIABLE FROM THE REMAINING EQUATIONS                          P1712  01429
C                                                                    P1712  01430
C      INTERCHANGE EQUATIONS I AND NN                                P1712  01431
C                                                                    P1712  01432
```

```
   28 IF(NN-I) 29,31,29                                        P1712   01433
   29 DO 30 J=NN,IUSE1                                         P1712   01434
      Z=G(I,J)                                                 P1712   01435
      G(I,J)=G(NN,J)                                           P1712   01436
      G(NN,J)=Z                                                P1712   01437
   30 CONTINUE                                                 P1712   01438
C                                                              P1712   01439
C     DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH P1712 01440
C     VARIABLE FROM THE REMAINING EQUATIONS                    P1712   01441
C                                                              P1712   01442
   31 K = NN + 1                                               P1712   01443
      DO 36 J = K, IUSE1                                       P1712   01444
      IF(G(NN,NN).EQ.0.)  GO TO 23                             P1712   01445
         G(NN,J) = G(NN,J) / G(NN,NN)                          P1712   01446
   36 CONTINUE                                                 P1712   01447
      IF(K-IUSE1) 88,45,38                                     P1712   01448
   88 DO 44 I = K,IUSE                                         P1712   01449
   40 DO 44 J = K, IUSE1                                       P1712   01450
         G(I,J) = G(I,J) - G(I,NN)*G(NN,J)                     P1712   01451
   44 CONTINUE                                                 P1712   01452
   45 CONTINUE                                                 P1712   01453
C                                                              P1712   01454
C     BACKSOLVE FOR THE VARIABLES                              P1712   01455
C                                                              P1712   01456
      K = IUSE                                                 P1712   01457
   47 J = K + 1                                                P1712   01458
C     X(K) = 0.000                                             P1712   01459
      X(K) = 0.0                                               P1712   01460
      SUM = 0.0                                                P1712   01461
      IF(IUSE - J) 51,48,48                                    P1712   01462
   48 DO 50 I = J,IUSE                                         P1712   01463
         SUM = SUM + G(K,I)* X(I)                              P1712   01464
   50 CONTINUE                                                 P1712   01465
   51 X(K) = G(K,IUSE1) - SUM                                  P1712   01466
      K = K - 1                                                P1712   01467
      IF (K) 67,151,47                                         P1712   01468
   23 IUSE = IUSE-1                                            P1712   01469
  151 RETURN                                                   P1712   01470
      END                                                      P1712   01471
```

```
      SUBROUTINE MOLIER                                                  P1712  01472
C                                                                        P1712  01473
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)        P1712  01474
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)   P1712  01475
     2,ICTN(13)                                                          P1712  01476
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)    P1712  01477
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)              P1712  01478
      COMMON/MISC/ERN,SUMN,TT,SU,ATOM(3,101),LLMT(15),BO(15),BOP(15,2)   P1712  01479
     1 ,TK,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712  01480
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)          P1712  01481
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  01482
     4 ,RHOP,RMW(15),TLN,JANF                                            P1712  01483
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSF,IPSP,MOLES,NP,NT,NPT,C,NS, P1712  01484
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ      P1712  01485
     2 ,IONS,KC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,TO2                    P1712  01486
      DO 91 IT = 1,26                                                    P1712  01487
      IF (T(IT).EQ. 0.) GO TO 95                                         P1712  01488
      NT = IT                                                            P1712  01489
   91 CONTINUE                                                           P1712  01490
C                                                                        P1712  01491
C     SET ASSIGNED P                                                     P1712  01492
C                                                                        P1712  01493
   95 DO 902 IP = 1,NP                                                   P1712  01494
      PP = P(IP)                                                         P1712  01495
C                                                                        P1712  01496
C     SET ASSIGNED T                                                     P1712  01497
C                                                                        P1712  01498
      DO 902 IT=1,NT                                                     P1712  01499
      TT = T(IT)                                                         P1712  01500
      CALL EQLBRM                                                        P1712  01501
      IF(TT.NE.0.)  GO TO 900                                            P1712  01502
      IF(NPT.EQ.0)  GO TO 1000                                           P1712  01503
  800 K = 0                                                              P1712  01504
      IF(IP.EQ.NP.AND.IT.EQ.NT.OR.TT.EQ.0.)  GO TO 860                   P1712  01505
      K = NPT                                                            P1712  01506
      IF(NPT.NE.13)  GO TO 870                                           P1712  01507
  860 WRITE (6,5)                                                        P1712  01508
    5 FORMAT(1H1,41X,48HTHERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED P1712  01509
     1    ,/43X,28H TEMPERATURES AND PRESSURES     ///  )                P1712  01510
      CALL OUT1                                                          P1712  01511
      WRITE (6,863)                                                      P1712  01512
  863 FORMAT (25HOTHERMODYNAMIC PROPERTIES//)                            P1712  01513
      CALL OUT2                                                          P1712  01514
      CALL OUT3                                                          P1712  01515
  865 IF(K.EQ.0) GO TO 1000                                              P1712  01516
      WRITE(6,868)                                                       P1712  01517
  868 FORMAT(1H1)                                                        P1712  01518
      NPT = 0                                                            P1712  01519
  870 NPT = NPT + 1                                                      P1712  01520
C                                                                        P1712  01521
C  SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT                         P1712  01522
C                                                                        P1712  01523
      DO 880 I = 1,NS                                                    P1712  01524
```

```
          EN(I,NPT) = EN(I,K)                              P1712  01525
      880 CONTINUE                                         P1712  01526
      902 CONTINUE                                         P1712  01527
     1000 RETURN                                           P1712  01526
          END                                              P1712  01529
```

```
      SUBROUTINE OUT1                                                  P1712   01530
C                                                                      P1712   01531
C     DOUBLE PRECISION G,X                                             P1712   01532
      LOGICAL EQL,FROZ ,TP,HP,SP,HPSP,TPSP,MOLES                       P1712   01533
C                                                                      P1712   01534
      DIMENSION NV(13),Z(10,3),HEAD(15),YX(5),YN(5)                    P1712   01535
C                                                                      P1712   01536
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)      P1712   01537
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) P1712   01538
     2 ,TOTN(13)                                                       P1712   01539
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)  P1712   01540
     1 ,CELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)            P1712   01541
      COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),BOP(15,2) P1712   01542
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AL(2),AM(2) P1712   01543
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)        P1712   01544
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712   01545
     4 ,RHCP,RMW(15),TLN,JANF                                          P1712   01546
      COMMON /DOUBLE/ G(28,21), X(20)                                  P1712   01547
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712   01548
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ    P1712   01549
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                  P1712   01550
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13) P1712   01551
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSG                            P1712   01552
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)    P1712   01553
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2       P1712   01554
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FO                      P1712   01555
      COMMON/CVOLUM/ VOLUMC,IMPETUS,IFLGGG                             P1712   01556
      COMMON/PRCENT/ FMOLE                                             P171201 00001
      REAL IMPETUS                                                     P1712   01557
C                                                                      P1712   01558
      EQUIVALENCE (V,NV),(Z,H0)                                        P1712   01559
C                                                                      P1712   01560
C     HEAD=(1H ,2A4,5  (A2,F8.5,3X),5  X,F7.5,F13.3,4X,A1,F10.2,F9.4)  P1712   01561
C                                                                      P1712   01562
      DATA HEAD/4H(1H ,4H,2A4,2H,5,4H(A2,,4HF8.5 ,4H,3X),2H,5 ,2HX,    P1712   01563
     1     ,4HF7.5 ,4H,F13 ,4H.3,4 ,4HX,A1 ,4H,F10 ,4H.2,F ,4H9.4)/    P1712   01564
      DATA FUEL/4HFUEL/,OXID/4HOXID/,ANT/3HANT/,OX/1HO/                P1712   01565
     1      ,YN/2H,1, 2H,2, 2H,3, 2H,4, 2H,5 /                         P1712   01566
     2      ,YX/3H,57,3H,44,3H,31,3H,18,2H,5 /                         P1712   01567
C                                                                      P1712   01568
      WRITE(6,4) KASE                                                  P1712   01569
    4 FORMAT(1H0,13A6,A2)                                              P1712   01570
    3 FORMAT (9H CASE NO. ,I5)                                         P1712   01571
      IF(.NOT.MOLES) WRITE(6,5)                                        P1712   01572
    5 FORMAT (77X,46HWT FRACTION  ENTHALPY  STATE    TEMP    DENSITY/  P1712   01573
     1 10X,16HCHEMICAL FORMULA,51X,21H(SEE NOTE)     CAL/MOL,10X,5HDEG K, P1712   01574
     2 4X,4HG/CC )                                                     P1712   01575
      IF(MOLES) WRITE(6,6)                                             P1712   01576
    6 FORMAT (84X,5HMOLES,8X,   33HENTHALPY  STATE   TEMP    DENSITY/  P1712   01577
     1 10X,16HCHEMICAL FORMULA,67X,7HCAL/MOL,10X,13HDEG K     G/CC )   P1712   01578
      DO 15 N=1,NREAC                                                  P1712   01579
      IF(FOX(N).EQ.FOX(N-1))GO TO 11                                   P1712   01580
      IF(FOX(N).NE.OX)GO TO 10                                         P1712   01581
```

```
          HD1 = CXID                                                  P1712  01582
          HD2 = ANT                                                   P1712  01583
          GO TO 11                                                    P1712  01584
       10 HD1 = FUEL                                                  P1712  01585
          HD2 = F8                                                    P1712  01586
       11 DO 13 J=1,5                                                 P1712  01587
          IF(ANUM(N,J).EQ.0.)GO TO 14                                 P1712  01588
       13 CONTINUE                                                    P1712  01589
          J=5                                                         P1712  01590
       14 J=J-1                                                       P1712  01591
          HEAD(3)=YN(J)                                               P1712  01592
          HEAD(7)=YX(J)                                               P1712  01593
          WRITE(6,HEAD)HD1,HD2,(NAME(N,JJ),ANUM(N,JJ),JJ=1,J),PECNT(N),ENTH( P1712  01594
         1N), FAZ(N),RTEMP(N),DENS(N)                                 P1712  01595
       15 CONTINUE                                                    P1712  01596
          WRITE(6,20) OF,FPCT,EQRAT,RHOP                              P1712  01597
       20 FORMAT (1H0,15X, 4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,  P1712  01598
         1  19HEQUIVALENCE RATIO= ,F7.4,4X,8HDENSITY=,F8.4//)         P1712  01599
    C                                                                 P1712  01600
          AGV = 9.80665                                               P1712  01601
          DO 25 I = 1,NPT                                             P1712  01602
          TOTN(I) = 0                                                 P1712  01603
          DO 25 J = 1,NS                                              P1712  01604
          TOTN(I) = TOTN(I) + EN(J,I)                                 P1712  01605
       25 CONTINUE                                                    P1712  01606
          FMT(4)= FMT(6)                                              P1712  01607
          RETURN                                                      P1712  01608
    C                                                                 P1712  01609
          ENTRY OUT2                                                  P1712  01610
    C                                                                 P1712  01611
    C   PRESSURE                                                      P1712  01612
    C                                                                 P1712  01613
          DO 55 I=1,NPT                                               P1712  01614
          K= 2*I+3                                                    P1712  01615
          FMT(K)= F4                                                  P1712  01616
          IF (PPP(I).GE.1.) FMT(K)=F3                                 P1712  01617
          IF (PPP(I).GE.10.) FMT(K)=F2                                P1712  01618
          IF (PPP(I).GE.100.) FMT(K)=F1                               P1712  01619
       55 CONTINUE                                                    P1712  01620
          WRITE (6,FMT) (FP(I),I=1,4),(PPP(J),J=1,NPT)                P1712  01621
    C                                                                 P1712  01622
    C   TEMPERATURE                                                   P1712  01623
    C                                                                 P1712  01624
          DO 65 I=1,NPT                                               P1712  01625
          NV(I)= TT(I)+.5                                             P1712  01626
       65 CONTINUE                                                    P1712  01627
          FMT(4)= FMT13                                               P1712  01628
          FMT(5)= FMT19                                               P1712  01629
          WRITE (6,FMT) (FT(I),I=1,4),(NV(J),J=1,NPT)                 P1712  01630
    C                                                                 P1712  01631
    C   ENTHALPY                                                      P1712  01632
    C                                                                 P1712  01633
          DO 75 I=1,NPT                                               P1712  01634
```

```
      V(I) = HSUM(I) * R
   75 CONTINUE
      FMT(5)= F8
      FMT(7)= F1
      WRITE (6,FMT)(FH(I),I=1,4),(V(J),J=1,NPT)
C
C     ENTROPY
C
      FMT(7)=F4
      DO 78 I = 1,NPT
      V(I) = SSUM(I) * R
   78 CONTINUE
      WRITE (6,FMT)(FS(I),I=1,4),(V(J),J=1,NPT)
      WRITE (6,80)
   80 FORMAT ( 1H )
C
C     MOLECULAR WEIGHT
C
      FMT(7)= F3
      WRITE (6,FMT)(FM(I),I=1,4),(WM(J),J=1,NPT)
C
C     (DLV/DLP)T
C
      FMT(7)=F5
      IF(EQL) WRITE(6,FMT)(FV(I),I=1,4),(DLVPT(J),J=1,NPT)
C
C     (DLV/DLT)P
C
      FMT(7)= F4
      IF(EQL) WRITE(6,FMT)(FD(I),I=1,4),(DLVTP(J),J=1,NPT)
C
C     HEAT CAPACITY
C
      DO 85  I=1,NPT
      V(I) = CPR(I) * R
   85 CONTINUE
      WRITE(6,FMT)(FC(I),I=1,4),(V(J),J=1,NPT)
C
C     GAMMA(S)
C
      WRITE(6,FMT)(FG(I),I=1,4),(GAMMAS(J),J=1,NPT)
C
C     SONIC VELOCITY
C
      FMT(7)= F1
      DO 95 I = 1,NPT
      SONVEL(I) = SQRT(RR*GAMMAS(I)*TTT(I)/WM(I))
   95 CONTINUE
      WRITE(6,FMT)(FL(I),I=1,4),(SONVEL(J),J=1,NPT)
      VOLUMC=GAMMAS(1)*TTT(1)
      IMPETUS=VOLUMC*2781./WM(1)
      RETURN
C
```

```
          ENTRY OUT3                                                      P1712    01688
          IF(.NOT.EQL)  GO TO 331                                         P1712    01689
C                                                                         P1712    01690
C     MOLE FRACTIONS - EQUILIBRIUM                                        P1712    01691
C                                                                         P1712    01692
          WRITE (6,80)                                                    P1712    01693
          FMT(7)= F9                                                      P1712    01694
          WRITE(6,310)                                                    P1712    01695
      310 FORMAT(15H0MOLE FRACTIONS //)                                   P1712    01696
          DO 330 K=1,NS                                                   P1712    01697
          DO 315 I=1,NPT                                                  P1712    01698
          V(I) = EN(K,I) /TOTN(I)                                         P1712    01699
      315 CONTINUE                                                        P1712    01700
          DO 316 I=1,NPT                                                  P1712    01701
          IF (V(I).GE.(5.E-6)) GO TO 320                                  P1712    01702
      316 CONTINUE                                                        P1712    01703
          GO TO 330                                                       P1712    01704
      320 WRITE (6,FMT) SUB(K,1),SUB(K,2),SUB(K,3),FB,(V(I),I=1,NPT)      P1712    01705
      330 CONTINUE                                                        P1712    01706
      331 WRITE(6,335)                                                    P1712    01707
      335 FORMAT(113H0ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MO P1712   01708
         1LE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS//) P1712   01709
          LINE= 0                                                         P1712    01710
          DO 350 K=1,NS                                                   P1712    01711
          DO 340 I=1,NPT                                                  P1712    01712
          IF ((EN(K,I)/TOTN(I)).GE.(5.E-6)) GO TO 343                     P1712    01713
      340 CONTINUE                                                        P1712    01714
          LINE= LINE+1                                                    P1712    01715
          Z(LINE,1)= SUB(K,1)                                             P1712    01716
          Z(LINE,2)= SUB(K,2)                                             P1712    01717
          Z(LINE,3)= SUB(K,3)                                             P1712    01718
      343 IF ((LINE.NE.10) .AND. K.NE.NS) GO TO 350                       P1712    01719
          IF (LINE.EQ.0) GO TO 1000                                       P1712    01720
          WRITE(6,345) (Z(LN,1),Z(LN,2),Z(LN,3),LN=1,LINE)                P1712    01721
      345 FORMAT (10(1X,3A4))                                             P1712    01722
          LINE= 0                                                         P1712    01723
      350 CONTINUE                                                        P1712    01724
          IF(.NOT.MOLES) WRITE(6,360)                                     P1712    01725
      360 FORMAT(78H0NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXI P1712   01726
         2DANT IN TOTAL OXIDANTS   )                                      P1712    01727
          WRITE(6,1100) PMOLE                                             P171201  00002
     1100 FORMAT(1H0,*VISCOSITY AND CONDUCTIVITY VALUES BASED ON *,F5.1,* PE P171201 00003
         1RCENT OF GAS MIXTURE*)                                          P171201  00004
     1000 RETURN                                                          P1712    01728
          END                                                             P1712    01729
```

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      SUBROUTINE RATIO                                                  P1712  01730
C                                                                       P1712  01731
C     (USED FOR AREA RATIO INTERPOLATION ONLY)                          P1712  01732
C                                                                       P1712  01733
C     DOUBLE PRECISION G,X                                              P1712  01734
      LOGICAL EQL, FROZ,TPSP                                            P1712  01735
C                                                                       P1712  01736
      DIMENSION PER(2,2),AI(13),APCP(13),AT(13),AMHT(13),RP(2),NV(13)   P1712  01737
     1 , RPP(2)                                                         P1712  01738
C                                                                       P1712  01739
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)       P1712  01740
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)  P1712  01741
     2,TCTN(13)                                                         P1712  01742
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)   P1712  01743
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)             P1712  01744
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),BU(15),BOP(15,2)  P1712  01745
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AC(2),AM(2) P1712  01746
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)         P1712  01747
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  01748
     4 ,RHOP,KMW(15),TLN,JANF                                           P1712  01749
      COMMON /DOUBLE/ G(20,21), X(20)                                   P1712  01750
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  01751
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ     P1712  01752
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),JREAC,IC,IQ2                   P1712  01753
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13) P1712  01754
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SS0                             P1712  01755
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)     P1712  01756
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2        P1712  01757
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0                       P1712  01758
C                                                                       P1712  01759
      EQUIVALENCE (V,NV)                                                P1712  01760
C                                                                       P1712  01761
      NBLO = NPT-2                                                      P1712  01762
      DO 22 J=3,NPT                                                     P1712  01763
      IF(PCP(J).GT.PCP(2))GO TO 30                                      P1712  01764
   22 CONTINUE                                                          P1712  01765
      GO TO 31                                                          P1712  01766
   30 NBLO=J-3                                                          P1712  01767
   31 DO 1200  ISONIC=1,2                                               P1712  01768
      LL = 1                                                            P1712  01769
      IF(ISONIC.EQ.2)  GO TO 34                                         P1712  01770
      IF(NSUB.EQ.0)  GO TO 1200                                         P1712  01771
      NAR = NSUB                                                        P1712  01772
      GO TO 36                                                          P1712  01773
   34 IF(NSUP.EQ.0)  GO TO 1200                                         P1712  01774
      NAR = NSUP                                                        P1712  01775
   36 DO 1100 I=1,NAR                                                   P1712  01776
      IF(ISONIC.EQ.2)  GO TO 40                                         P1712  01777
      IF(NBLO.LE.1) GO TO 1100                                          P1712  01778
      K=2+NBLO                                                          P1712  01779
      DO 38 JJ=4,K                                                      P1712  01780
      J=JJ                                                              P1712  01781
      V(LL) = SUBAR(I)                                                  P1712  01782
```

```
      IF(V(LL).GE.AEAT(J))  GO TO 56                              P1712  01783
   38 CONTINUE                                                    P1712  01784
      GO TO 56                                                    P1712  01785
   40 IF(NPT-NBLO.LE.3)   GO TO 1100                              P1712  01786
      V(LL) = SUPAR(I)                                            P1712  01787
      K=4+NBLO                                                    P1712  01788
      DO 42 JJ=K,NPT                                              P1712  01789
      J=JJ                                                        P1712  01790
      IF(V(LL).LE.AEAT(J))   GO TO 56                             P1712  01791
   42 CONTINUE                                                    P1712  01792
      IF(V(LL).GE.AEAT(J)*3.)   GO TO 85                          P1712  01793
   56 KJ = J-1                                                    P1712  01794
      K = KJ                                                      P1712  01795
      DO 64 JJ=1 2                                                P1712  01796
      IF(CPR(K).NE.0.)   GO TO 63                                 P1712  01797
      WRITE(6,62)K                                                P1712  01798
   62 FORMAT(17HOCANNOT USE POINT,I2,3X,4HCP=0 )                  P1712  01799
      GO TO 1100                                                  P1712  01800
   63 PER(JJ,1)=-1./(CPR(K)*WM(K))                                P1712  01801
      IF (EQL) PER(JJ,1) =   PER(JJ,1)*DLVTP(K)                   P1712  01802
      PER(JJ,2)=    TTT(K)/(2.*WM(K)*(HSUM(1)-HSUM(K)))           P1712  01803
      RP(JJ) = 1./(1./GAMMAS(K)-PER(JJ,2))                        P1712  01804
      IF(EQL)RPP(JJ) = 1.+DLVPT(K)+(1.-DLVTP(K))*PER(JJ,1)        P1712  01805
      K = KJ + 1                                                  P1712  01806
   64 CONTINUE                                                    P1712  01807
      AMWT(LL) = WM(1)                                            P1712  01808
      CALL SET(PCP(KJ),RP(1),AEAT(KJ),V(LL),    APCP(LL))         P1712  01809
      CALL SET(TTT(KJ),PER(1,1),PCP(KJ),APCP(LL),AT(LL))          P1712  01810
      IF(EQL)CALL SET (WM(KJ),RPP(1),PCP(KJ),APCP(LL),AMWT(LL))   P1712  01811
      K = KJ                                                      P1712  01812
      DO 74 JJ=1,2                                                P1712  01813
      G(JJ,7)=SPIM(K)**2                                          P1712  01814
      G(JJ+2,7)=2.*G(JJ,7)*PER(JJ,2)                              P1712  01815
      G(JJ+4,7)=(1.-GAMMAS(K))/GAMMAS(K)*G(JJ+2,7)                P1712  01816
      G(JJ,1)=1.                                                  P1712  01817
      G(JJ+2,1)= 0                                                P1712  01818
      G(JJ+4,1)=0                                                 P1712  01819
      G(JJ,2)=ALOG(PCP(K))                                        P1712  01820
      G(JJ+2,2)=1.                                                P1712  01821
      G(JJ+4,2)=0                                                 P1712  01822
      DO 70 M=3,6                                                 P1712  01823
      MXP=M-1                                                     P1712  01824
      G(JJ,M)=G(JJ,2)**MXP                                        P1712  01825
      MXP=MXP-1                                                   P1712  01826
      G(JJ+2,M)=G(JJ,2)**MXP*FLOAT(M-1)                           P1712  01827
      G(JJ+4,M)=G(JJ+2,M)/G(JJ,2)*FLOAT(M-2)                      P1712  01828
   70 CONTINUE                                                    P1712  01829
      K = KJ + 1                                                  P1712  01830
   74 CONTINUE                                                    P1712  01831
      IMAT = 6                                                    P1712  01832
      CALL MGAUSD                                                 P1712  01833
      AI(LL)= X (1)                                               P1712  01834
      DO 84 JJ=2,6                                                P1712  01835
```

```
      AI(LL)=AI(LL)+ X (JJ)*ALOG(APCP(LL))**(JJ-1)                 P1712  01836
   84 CONTINUE                                                      P1712  01837
      IF(AI(LL).LE.0.)GO TO 85                                      P1712  01838
      AI(LL) = AI(LL)**.5                                           P1712  01839
      GO TO 86                                                      P1712  01840
   85 LL = LL - 1                                                   P1712  01841
   86 IF(LL.GE.15.OR.I.GE.NAR) GO TO 90                             P1712  01842
      LL = LL+1                                                     P1712  01843
      GO TO 1100                                                    P1712  01844
C                                                                   P1712  01845
C     OUTPUT                                                        P1712  01846
C                                                                   P1712  01847
   90 IF(EQL) WRITE (6,87)                                          P1712  01848
   87 FORMAT(1H1/20X,* THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING E P171201 00005
     1QUILIBRIUM COMPOSITION DURING EXPANSION*//)                   P1712  01850
      IF (.NOT.EQL) WRITE (6,88)                                    P1712  01851
   88 FORMAT(1H1/20X,* THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING F P171201 00006
     1ROZEN COMPOSITION DURING EXPANSION*//)                        P1712  01853
      IF (TPSM) WRITE (6,99)                                        P1712  01854
   99 FORMAT (52X,28HAT AN ASSIGNED TEMPERATURE      )              P1712  01855
      WRITE (6,91)                                                  P1712  01856
   91 FORMAT (52X,24HFOR ASSIGNED AREA RATIOS     //)               P1712  01857
      PC= P(1)*14.696E06                                            P1712  01858
      WRITE(6,191)PC                                                P1712  01859
  191 FORMAT(9H P     = ,F8.1,5H PSIA)                              P1712  01860
      CALL OUT1                                                     P1712  01861
      IF(ISONIC.EQ.1) WRITE(6,33)                                   P1712  01862
   33 FORMAT(18H0SUBSONIC FLOW       //)                            P1712  01863
      IF (ISONIC.EQ.2) WRITE (6,35)                                 P1712  01864
   35 FORMAT(18H0SUPERSONIC FLOW     //)                            P1712  01865
C                                                                   P1712  01866
C     AREA RATIO                                                    P1712  01867
C                                                                   P1712  01868
      FMT(6)= FMT(8)                                                P1712  01869
      FMT(4)= FMT(6)                                                P1712  01870
      DO 92 M=1,LL                                                  P1712  01871
      K= 2*M+3                                                      P1712  01872
      FMT(K)= F3                                                    P1712  01873
      IF(V(M).GE.10.) FMT(K)=F2                                     P1712  01874
      IF(V(M).GE.100.) FMT(K)=F1                                    P1712  01875
   92 CONTINUE                                                      P1712  01876
      WRITE(6,FMT) FA1,FA2,FB,FB,(V(M),M=1,LL)                      P1712  01877
C                                                                   P1712  01878
C     VACUUM SPECIFIC IMPULSE AND SPECIFIC IMPULSE                  P1712  01879
C                                                                   P1712  01880
      DO 93 M=1,LL                                                  P1712  01881
      V(M)=AI(M)+CSTR*V(M)/(32.174* APCP(M))                        P1712  01882
   93 CONTINUE                                                      P1712  01883
      FMT(4)= FMT13                                                 P1712  01884
      FMT(5)= F8                                                    P1712  01885
      FMT(7)= F1                                                    P1712  01886
      WRITE(6,FMT) (FA(N),N=1,4), (V(M),M=1,LL)                     P1712  01887
      WRITE(6,FMT) (FI(N),N=1,4), (AI(M),M=1,LL)                    P1712  01888
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      C                                                                 P1712  01889
      C     C*                                                          P1712  01890
      C                                                                 P1712  01891
            FMT(5)= FMT19                                               P1712  01892
            DO 94 M=1,LL                                                P1712  01893
            NV(M)=CSTR +.5                                              P1712  01894
         94 CONTINUE                                                    P1712  01895
            WRITE(6,FMT)  (FR(N),N=1,4), (NV(M),M=1,LL)                 P1712  01896
      C                                                                 P1712  01897
      C     CF - THRUST COEFFICIENT                                     P1712  01898
      C                                                                 P1712  01899
            DO 95 M=1,LL                                                P1712  01900
            V(M)=AI(M)*32.174/CSTR                                      P1712  01901
         95 CONTINUE                                                    P1712  01902
            FMT(5)= F8                                                  P1712  01903
            FMT(7)= F3                                                  P1712  01904
            WRITE(6,FMT)  FC1,F8,F8,F8,(V(M),M=1,LL)                    P1712  01905
            WRITE(6,96)                                                 P1712  01906
         96 FORMAT(1H )                                                 P1712  01907
      C                                                                 P1712  01908
      C     PRESSURE RATIO                                              P1712  01909
      C                                                                 P1712  01910
            FMT(4)= FMT(6)                                              P1712  01911
            DO 97 M=1,LL                                                P1712  01912
            K= 2*M+3                                                    P1712  01913
            FMT(K)= F3                                                  P1712  01914
            IF(APCP(M).GE.1000.) FMT(K)=F2                              P1712  01915
            IF(APCP(M).GE.10000.) FMT(K)=F1                             P1712  01916
         97 CONTINUE                                                    P1712  01917
      C                                                                 P1712  01918
      C     PRESSURE                                                    P1712  01919
      C                                                                 P1712  01920
            WRITE(6,FMT)  FR1,F8,F8,F8,(APCP(M),M=1,LL)                 P1712  01921
            DO 98 M=1,LL                                                P1712  01922
            K= 2*M+3                                                    P1712  01923
            V(M)=P(1)/APCP(M)                                           P1712  01924
            FMT(K)= F4                                                  P1712  01925
            IF(V(M).GE.1.) FMT(K)=F3                                    P1712  01926
            IF(V(M).GE.10.) FMT(K)=F2                                   P1712  01927
            IF(V(M).GE.100.) FMT(K)=F1                                  P1712  01928
         98 CONTINUE                                                    P1712  01929
            WRITE(6,FMT)  (FP(N),N=1,4), (V(M),M=1,LL)                  P1712  01930
      C                                                                 P1712  01931
      C     TEMPERATURE                                                 P1712  01932
      C                                                                 P1712  01933
            DO 101 M=1,LL                                               P1712  01934
            NV(M)=AT(M)+.5                                              P1712  01935
        101 CONTINUE                                                    P1712  01936
            FMT(4)= FMT13                                               P1712  01937
            FMT(5)= FMT19                                               P1712  01938
            WRITE(6,FMT)  (FT(N),N=1,4), (NV(M),M=1,LL)                 P1712  01939
      C                                                                 P1712  01940
      C     ENTHALPY                                                    P1712  01941
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      C                                                           P1712   01942
                                                                  P1712   01943
            FMT(5)= F8                                            P1712   01944
            FMT(7)= F1                                            P1712   01945
            DO 104 M=1,LL                                         P1712   01946
            V(M)= MSUM(1)*R-1000.*(AI(M)/294.98)**2               P1712   01947
        104 CONTINUE                                              P1712   01948
            WRITE(6,FMT) (FP(N),N=1,4), (V(M),M=1,LL)             P1712   01949
      C                                                           P1712   01950
      C     ENTROPY                                               P1712   01951
      C                                                           P1712   01952
            FMT(7)=F4                                             P1712   01953
            V(1) = SSUM(2)*R                                      P1712   01954
            DO 106 M=1,LL                                         P1712   01955
            V(M) = V(1)                                           P1712   01956
        106 CONTINUE                                              P1712   01957
            WRITE(6,FMT) (FS(N),N=1,4), (V(M),M=1,LL)             P1712   01958
      C                                                           P1712   01959
      C     MOLECULAR WEIGHT                                      P1712   01960
      C                                                           P1712   01961
            FMT(7)=F3                                             P1712   01962
            WRITE(6,FMT) (FM(N),N=1,4), (AMNT(M),M=1,LL)          P1712   01963
       1100 CONTINUE                                              P1712   01964
       1200 CONTINUE                                              P1712   01965
            RETURN                                                P1712   01966
            END
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      SUBROUTINE REACT                                                  P1712   01967
C                                                                       P1712   01968
C                                                                       P1712   01969
C     DOUBLE PRECISION G,X                                              P1712   01970
      LOGICAL HP,SP,TP,IDEBUG,CONVG,NEWR,IONS,MOLES,EQL,FROZ            P1712   01971
C                                                                       P1712   01972
      DIMENSION ANAME(15,5),V(15)                                       P1712   01973
C                                                                       P1712   01974
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)  P1712   01975
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,MSUB0,AC(2),AM(2) P1712   01976
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)         P1712   01977
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712   01978
     4 ,RHOP,RMW(15),TLN,JANF                                           P1712   01979
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712   01980
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ      P1712   01981
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                   P1712   01982
C                                                                       P1712   01983
      EQUIVALENCE (NAME,ANAME)                                          P1712   01984
C                                                                       P1712   01985
      DATA MOL/1HM/,OX/1HO/,LANK/1H /,IZERO/2H00/                       P1712   01986
C                                                                       P1712   01987
      WRITE(6,9000)                                                     P1712   01988
 9000 FORMAT(1H ,*REACTANTS*)                                           P1712   01989
      DO 10 K=1,2                                                       P1712   01990
      WP(K)=0.                                                          P1712   01991
      HPP(K)=0.                                                         P1712   01992
      RHO(K)=0.                                                         P1712   01993
      VPLS(K)=0.                                                        P1712   01994
      VMIN(K)=0.                                                        P1712   01995
      AC(K)=0.                                                          P1712   01996
      AM(K)=0.                                                          P1712   01997
      DO 8 J=1,15                                                       P1712   01998
      LLMT(J)=0                                                         P1712   01999
      B0P(J,K)=0.                                                       P1712   02000
    8 CONTINUE                                                          P1712   02001
   10 CONTINUE                                                          P1712   02002
      N=1                                                               P1712   02003
      L=1                                                               P1712   02004
      NREACS=NREAC                                                      P1712   02005
      IF(NREAC.GT.16) NREAC=16                                          P1712   02006
      DO 200 N=1,NREAC                                                  P1712   02007
   20 READ(5,21)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ(N) P1712   02008
     1 ,RTEMP(N),FOX(N),DENS(N)                                         P1712   02009
   21 FORMAT(5(A2,F7.5),F7.5,A1,F9.5,A1,F8.5,A1,F8.5)                   P1712   02010
      IF(NAME(N,1).EQ.LANK) GO TO 200                                   P1712   02011
      IF(L.EQ.0)GO TO 20                                                P1712   02012
      WRITE (6,31)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ P1712   02013
     1  (N),RTEMP(N),FOX(N),DENS(N)                                     P1712   02014
   31 FORMAT(1X,5(A2,1X,F7.4,2X),F9.4,2X,A1,F11.2,2X,A1,2X,F8.3,2X,     P1712   02015
     1A1,3X,F8.5)                                                       P1712   02016
   35 IF(MOLE.EQ.MOL) MOLES=.TRUE.                                      P1712   02017
      K=2                                                               P1712   02018
      IF(FOX(N).EQ.OX)K=1                                               P1712   02019
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      DO 38 J=1,15                                           P1712   02020
      DATA(J) = 0.                                           P1712   02021
   38 CONTINUE                                               P1712   02022
      RM=0.                                                  P1712   02023
      GO 100 JJ=1,5                                          P1712   02024
      IF(ANUM(N,JJ).EC.0.)GO TO 101                          P1712   02025
      DO 41 J=1,15                                           P1712   02026
      NJ = J                                                 P1712   02027
      IF(LLMT(J).EQ.0) GO TO 45                              P1712   02028
      IF(NAME(N,JJ).EQ.LLMT(J))GO TO 46                      P1712   02029
   41 CONTINUE                                               P1712   02030
   45 L = NJ                                                 P1712   02031
      LLPT(J)=NAME(N,JJ)                                     P1712   02032
   46 DO 48 KK=1,101                                         P1712   02033
      IF(ATOM(1,KK).EQ.ANAME(N,JJ))GO TO 50                  P1712   02034
   48 CONTINUE                                               P1712   02035
      L=0                                                    P1712   02036
      GC TO 20                                               P1712   02037
   50 RM=RM+ANUM(N,JJ)*ATOM(2,KK)                            P1712   02038
      V(J)=ATOM(3,KK)                                        P1712   02039
      DATA(J)=ANUM(N,JJ)                                     P1712   02040
  100 CONTINUE                                               P1712   02041
  101 PCNT=PECNT(N)                                          P1712   02042
      IF(MOLES) PCNT=PCNT*RM                                 P1712   02043
      WP(K)=WP(K) + PCNT                                     P1712   02044
      IF(NAME(N,5).NE.IZERO)HPP(K)=HPP(K)+ENTH(N)*PCNT/RM    P1712   02045
      AM(K)=AM(K)+PCNT/RM                                    P1712   02046
      DO 110  J=1,L                                          P1712   02047
      BOP(J,K)=DATA(J)*PCNT/RM +BOP(J,K)                     P1712   02048
  110 CONTINUE                                               P1712   02049
      IF(DENS(N).NE.0.)GO TO 115                             P1712   02050
      GO TO 117                                              P1712   02051
  115 RHO(K)=RHO(K)+PCNT/DENS(N)                             P1712   02052
  117 RMK(N) = RM                                            P1712   02053
  200 CONTINUE                                               P1712   02054
      IF(NREACS.LE.16) GO TO 1205                            P1712   02055
      NRAC=NREACS-16                                         P1712   02056
      DO 1200 I=1,NRAC                                       P1712   02057
 1200 READ(5,21) JUNK                                        P1712   02058
 1205 IF(L.EQ.0) GO TO 1000                                  P1712   02059
      IF(L.EQ.0) GO TO 1000                                  P1712   02060
      DO 220 K=1,2                                           P1712   02061
      IF(WP(K).EQ.0.)GO TO 220                               P1712   02062
      HPP(K)=HPP(K)/WP(K)                                    P1712   02063
      AM(K) = WP(K)/AM(K)                                    P1712   02064
      IF(RHO(K).NE.0.)RHO(K)=WP(K)/RHO(K)                    P1712   02065
      DO 215 J=1,L                                           P1712   02066
      BOP(J,K)=BOP(J,K)/WP(K)                                P1712   02067
      IF(V(J).LT.0.)VMIN(K)= VMIN(K)+BOP(J,K)*V(J)           P1712   02068
      IF(V(J).GT.0.)VPLS(K)=VPLS(K)+BOP(J,K)*V(J)            P1712   02069
  215 CONTINUE                                               P1712   02070
      IF(MOLES) GO TO 220                                    P1712   02071
      DO 218 N=1,NREAC                                       P1712   02072
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      IF(FOX(N).EQ.OX.AND.K.EQ.2)  GO TO 218          P1712  02073
      IF(FOX(N).NE.OX.AND.K.EQ.1)  GO TO 218          P1712  02074
      PECWT(N) = PECWT(N)/WP(K)                        P1712  02075
                                                       P1712  02076
  218 CONTINUE                                         P1712  02077
  220 CONTINUE                                         P1712  02078
      NEWR=.TRUE.                                      P1712  02079
      DO 230 N = 1,NREAC                               P1712  02080
      IF (DENS(N).NE.C.) GO TO 230                     P1712  02081
      RHO (1) = 0.                                     P1712  02082
      GO TO 1000                                       P1712  02083
  230 CONTINUE                                         P1712  02084
 1000 RETURN                                           P1712  02085
      END
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      SUBROUTINE RKTOUT                                                 P1712  02086
C                                                                       P1712  02087
C     ROCKET PERFORMANCE PERAMETERS                                     P1712  02088
C                                                                       P1712  02089
C                                                                       P1712  0209C
      LOGICAL EQL,FROZ ,TP,HP,SP,HPSP,TPSP,SHOCK                        P1712  02091
C                                                                       P1712  02092
      DIMENSION NV(13),Z(10,4)                                          P1712  02093
      DIMENSION VELOC(13)                                               P1712  02094
C                                                                       P1712  02095
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)       P1712  02096
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)  P1712  02097
     2 ,TCTN(13)                                                        P1712  02098
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)   P1712  02099
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)             P1712  02100
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)  P1712  02101
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,TR,HSUB0,AC(2),AM(2) P1712  02102
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)         P1712  02103
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  02104
     4 ,RHOP,RMW(15),TLN,JANF                                           P1712  02105
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  02106
     1  FMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ     P1712  02107
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                   P1712  02108
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13) P1712  02109
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSO                             P1712  02110
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)     P1712  02111
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2        P1712  02112
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0                       P1712  02113
      COMMON/CVOLUM/ VOLUMC,IMPETUS,IFLGGG                              P1712  02114
      REAL IMPETUS                                                      P1712  02115
C                                                                       P1712  02116
      EQUIVALENCE (V,NV),(Z,H0)                                         P1712  02117
C                                                                       P1712  02118
      DATA EXIT/4HEXIT/                                                 P1712  02119
C                                                                       P1712  02120
      IF(EQL) WRITE (6,37)                                              P1712  02121
   37 FORMAT(1H1/20X,* THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING E P171201 00007
     1QUILIBRIUM COMPOSITION DURING EXPANSION        *//)               P1712  02123
      IF (.NOT.EQL) WRITE (6,38)                                        P1712  02124
   38 FORMAT(1H1/20X,* THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING F P171201 00008
     1ROZEN COMPOSITION DURING EXPANSION        *//)                    P1712  02126
      IF (TPSP) WRITE (6,737)                                           P1712  02127
  737 FORMAT (52X,28HAT AN ASSIGNED TEMPERATURE       )                 P1712  02128
      V(1) = PPP(1)*14.696006                                           P1712  02129
      WRITE (6,40) V(1)                                                 P1712  02130
   40 FORMAT(5H PC = ,F8.1,5H PSIA)                                     P1712  02131
      CALL OUT1                                                         P1712  02132
      NEX = NPT - 2                                                     P1712  02133
      DO 862 I = 1,NEX                                                  P1712  02134
  862 V(I) = EXIT                                                       P1712  02135
      WRITE(6,48) (V(I),I=1,NEX)                                        P1712  02136
   48 FORMAT(1H0,16X,16HCHAMBER   THROAT  ,11(5X,A4))                   P1712  02137
C                                                                       P1712  02138
```

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      C      PRESSURE RATIOS                                     P1712   02139
      C                                                          P1712   02140
             DO 45 I=1,NPT                                       P1712   02141
             K= 2*I+3                                            P1712   02142
             FMT(K)= F3                                          P1712   02143
             IF (PCP(I).GE.1000.) FMT(K)=F2                      P1712   02144
             IF (PCP(I).GE.10000.)FMT(K)=F1                      P1712   02145
             IF (PCP(I).GE.1000000.)FMT(K) = F0                  P1712   02146
          45 CONTINUE                                            P1712   02147
             WRITE (6,FMT) FR1,FB,FB,FB,(PCP(J),J=1,NPT)         P1712   02148
             CALL OUT2                                           P1712   02149
      C                                                          P1712   02150
             AGV = 9.80665                                       P1712   02151
             DO 202 K=2,NPT                                      P1712   02152
             SPIM(K) = (2.*RR*(HSUM(1)-HSUM(K)))**.5/AGV         P1712   02153
      C                                                          P1712   02154
      C   AW (A/W) IN UNITS OF SEC/ATM                           P1712   02155
      C                                                          P1712   02156
             AW = RR*TTT(K)/(PPP(K)*          WM(K)*SPIM(K)*AGV**2)  P1712   02157
             IF(K.NE.2)GO TO 200                                 P1712   02158
             AWT=AW                                              P1712   02159
             CSTR=32.174*P(1)*AWT                                P1712   02160
         200 AEAT(K)=AW/AWT                                      P1712   02161
             VACI(K)=SPIM(K)+PPP(K)*AW                           P1712   02162
             IF (SONVEL(K).NE.0.) VMOC(K)=SPIM(K)*AGV/SONVEL(K)  P1712   02163
             NV(K)= CSTR + .5                                    P1712   02164
         202 CONTINUE                                            P1712   02165
      C                                                          P1712   02166
      C   MACH NUMBER                                            P1712   02167
      C                                                          P1712   02168
             VMOC(1)=0.                                          P1712   02169
             IF(GAMMAS(2).EQ.0.) VMOC(2)=0.                      P1712   02170
             FMT(7) = F3                                         P1712   02171
             WRITE(6,FMT)(FN(I),I=1,4),(VMOC(J),J=1,NPT)         P1712   02172
      C                                                          P1712   02173
      C   VELOCITY                                               P1712   02174
      C                                                          P1712   02175
             DO 1202 I=1,NPT                                     P1712   02176
             VELOC(I)=SONVEL(I)*VMOC(I)*3.280840                 P1712   02177
        1202 CONTINUE                                            P1712   02178
             WRITE(6,1203)(VELOC(I),I=1,NPT)                     P1712   02179
        1203 FORMAT(1H ,*VEL, FT/SEC   *,13F9.1)                 P1712   02180
             CALL VISCON(NS,NPT,SUB,EN,TOTN,TTT)                 P171201 00009
             IF(IFLGGG.GT.0) GO TO 203                           P1712   02181
      C                                                          P1712   02182
      C   CONSTANT VOLUME AND IMPETUS                            P1712   02183
      C                                                          P1712   02184
             IVOLUMC=VOLUMC+.5                                   P1712   02185
             WRITE(6,9000) IVOLUMC,IMPETUS                       P1712   02186
        9000 FORMAT(1H ,*T, CV, DEG K*,6X,I5/1H ,*IMPETUS       *,F7.0)  P1712   02187
         203 WRITE(6,208)                                        P1712   02188
         208 FORMAT (1H )                                        P1712   02189
      C                                                          P1712   02190
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C     C                                                           P1712  02191
C                                                                 P1712  02192
      FMT(4) = FMT9X                                              P1712  02193
      FMT(5) = FMT13                                              P1712  02194
      FMT(6) = FMTI9                                              P1712  02195
      FMT(7) = F8                                                 P1712  02196
      WRITE(6,FMT)(FR(I),I=1,4),(NV(J),J=2,NPT)                   P1712  02197
C                                                                 P1712  02198
C   CF - THRUST COEFICIENT                                        P1712  02199
C                                                                 P1712  02200
      FMT(6) = FMT(8)                                             P1712  02201
      FMT(7) = F3                                                 P1712  02202
      DO 212  I=2,NPT                                             P1712  02203
  212 V(I)=32.174*SPIM(I)/CSTR                                    P1712  02204
      WRITE(5,FMT)FC1,F8,F8,F8,(V(J),J=2,NPT)                     P1712  02205
C                                                                 P1712  02206
C   AREA RATIO                                                    P1712  02207
C                                                                 P1712  02208
      FMT(5) = F8                                                 P1712  02209
      DO 214 I = 2,NPT                                            P1712  02210
      K = 2*I+3                                                   P1712  02211
      FMT(K) = F4                                                 P1712  02212
      IF (AEAT(I).GE.1.) FMT(K) = F3                              P1712  02213
      IF (AEAT(I).GE.10.) FMT(K) = F2                             P1712  02214
      IF (AEAT(I).GE.100.) FMT(K) = F1                            P1712  02215
  214 CONTINUE                                                    P1712  02216
      WRITE(6,FMT)FA1,FA2,F8,F8,(AEAT(J),J=2,NPT)                 P1712  02217
C                                                                 P1712  02218
C   VACUUM IMPULSE                                                P1712  02219
C                                                                 P1712  02220
      FMT(5) = FMT13                                              P1712  02221
      FMT(7) = F1                                                 P1712  02222
      WRITE(6,FMT)(FA(I),I=1,4),(VASI(J),J=2,NPT)                 P1712  02223
C                                                                 P1712  02224
C   SPECIFIC IMPULSE                                              P1712  02225
C                                                                 P1712  02226
      WRITE(6,FMT)(FI(I),I=1,4),(SPIM(J),J=2,NPT)                 P1712  02227
      WRITE (6,208)                                               P1712  02228
      FMT(4) = F8                                                 P1712  02229
      FMT(5) = FMT13                                              P1712  02230
      FMT(7) = F5                                                 P1712  02231
      IF(EQL)  GO TO 312                                          P1712  02232
      WRITE(6,310)                                                P1712  02233
  310 FORMAT(15HOMOLE FRACTIONS //)                               P1712  02234
C                                                                 P1712  02235
C   MOLE FRACTIONS - FROZEN                                       P1712  02236
C                                                                 P1712  02237
      LINE = 0                                                    P1712  02238
      DO 430 K =1,NS                                              P1712  02239
      V(LINE+1) = EN(K,1)/TOTN(1)                                 P1712  02240
      IF (V(LINE+1).LT.(5.E-6))  GO TO 424                        P1712  02241
      LINE = LINE+1                                               P1712  02242
      Z(LINE,1) = SUB(K,1)                                        P1712  02243
```

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      Z(LINE,2) = [illegible]3(K,2)                                 P1712   02244
      Z(LINE,3) = SUB(K,3)                                          P1712   02245
      Z(LINE,4) = V(LINE)                                           P1712   02246
  424 IF (LINE.NE.4.AND.K.NE.NS)  GO TO 430                         P1712   02247
      IF (LINE.EQ.0)  GO TO 312                                     P1712   02248
      WRITE (6,426) (Z(LN,1),Z(LN,2),Z(LN,3),Z(LN,4),LN=1,LINE)     P1712   02249
  426 FORMAT (1H ,4(3A4,F9.5,7X))                                   P1712   02250
      LINE = 0                                                      P1712   02251
  430 CONTINUE                                                      P1712   02252
  312 CALL OUT3                                                     P1712   02253
 1000 RETURN                                                        P1712   02254
      END                                                           P1712   02255
```

```
      SUBROUTINE ROCKET
C
C
C     ROCKET PERFORMANCE
C     EITHER HPSP OR TPSP IS TRUE
C
      LOGICAL HP,SP,TP,IDEBUG,NEWR ,IONS,MOLES,FROZ,EQL,LOGV,HPSP,TPSP
C
      DIMENSION AA(2),BB(2),CC(2)
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2,TCTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,CELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),B0(15),BOP(15,2)
     1 ,TN,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHCP,RMW(15),TLN,JANF
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TSP,MOLES,NP,NT,NPT,L,NS,
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSD
      COMMON/CVOLUM/ VOLUMC,IMPETUS,IFLGGG
      REAL IMPETUS
C
      NAMELIST/RKTINP/EQL,FROZ,SUBAR,SUPAR,PCP
C
      ITM = 0
      IFLGGG=0
  210 DO 300 I=1,26
      PCP(I)= 0.
      SUBAR(I) = 0.
  300 CONTINUE
      HPSP = .TRUE.
      HP = .TRUE.
      TPSP = .FALSE.
      EQL = .TRUE.
      FROZ = .TRUE.
      READ (5,RKTINP)
      IF (T(1).EQ.0.)  GO TO 302
      TPSP = .TRUE.
      TP = .TRUE.
      HPSP = .FALSE.
      GO TO 303
  302 T(1) = 3800.
  303 IF (PCP(1).NE.0.)  GO TO 306
      DO 305  I=1,NP
      K = NP-I+2
      P(K) = P(K-1)
  305 CONTINUE
```

```
      GO TO 311                                         P1712  02309
  308 NP= 2                                             P1712  02310
      DO 310 I=1,24                                     P1712  02311
      IF (I.GT.2) GO TO 309                             P1712  02312
      IF ((PCP(I).EQ.0.).OR.PCP(I).EQ.1.) GO TO 310     P1712  02313
  309 IF (PCP(I).EQ.0.) GO TO 311                       P1712  02314
      NP = NP + 1                                       P1712  02315
      P(NP) = P(1)/PCP(I)                               P1712  02316
  310 CONTINUE                                          P1712  02317
  311 NSUB=0                                            P1712  02318
      NSUP = 0                                          P1712  02319
      DO 320  I=1,13                                    P1712  02320
      IF(SUBAR(I).NE.0.)NSUB=NSUB+1                     P1712  02321
      IF(SUPAR(I).NE.0.)NSUP=NSUP+1                     P1712  02322
  320 CONTINUE                                          P1712  02323
      WRITE (6,RKTINP)                                  P1712  02324
      SS0 = 0.                                          P1712  02325
      ITROT= 3                                          P1712  02326
      TT = T(1)                                         P1712  02327
C                                                       P1712  02328
C     SET ASSIGNED P                                    P1712  02329
C                                                       P1712  02330
      DO 902 IP = 1,NP                                  P1712  02331
      PP = P(IP)                                        P1712  02332
      CALL EQLBRM                                       P1712  02333
      T(NPT) = TT                                       P1712  02334
      IF(TT.NE.0.)  GO TO 333                           P1712  02335
      IF(NPT.EQ.0)  GO TO 1000                          P1712  02336
      GO TO 900                                         P1712  02337
  333 PCP(NPT) = P(1)/PP                                P1712  02338
      IF(IP.GT.1)  GO TO 195                            P1712  02339
C                                                       P1712  02340
C     COMBUSTION CHAMBER                                P1712  02341
C                                                       P1712  02342
      TP = .FALSE.                                      P1712  02343
      HP = .FALSE.                                      P1712  02344
      SP = .TRUE.                                       P1712  02345
      S0 = SSUM(1)                                      P1712  02346
      PCP(2)=((GAMMAS(1)+1.)/2.)**(GAMMAS(1)/(GAMMAS(1)-1.))   P1712  02347
      P(2) = P(1)/PCP(2)                                P1712  02348
      TT = 2.*TT/(GAMMAS(1)+1.)                         P1712  02349
      GO TO 900                                         P1712  02350
  195 IF(IP.GT.2) GO TO 900                             P1712  02351
C                                                       P1712  02352
C     THROAT                                            P1712  02353
C                                                       P1712  02354
  190 IF(ITH.NE.2)  GO TO 191                           P1712  02355
      ITH = 0                                           P1712  02356
      GAMMAS(2) = 0.                                    P1712  02357
      GO TO 900                                         P1712  02358
  191 DH = HSUM(1)-HSUM(2)                              P1712  02359
      DHSTAR = DH-GAMMAS(2)*TT*ENN/2.                   P1712  02360
      IF (IDEBUG) WRITE(6,923)DHSTAR,HSUM(1),HSUM(2),PCP(2)   P1712  02361
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```
  923 FORMAT(4E25.8)                                            P1712  02362
      CH = DHSTAR/DH                                            P1712  02363
      IF(DH.LT.0.)  DH=-DH                                      P1712  02364
      IF(DH.LE.0.4E-4.OR.ITROT.EQ.0)  GC TO 900                 P1712  02365
      IF(JSOL.NE.0) ITH =1                                      P1712  02366
      IF (JSOL.EQ.0.AND.ITH.EQ.1) ITH=2                         P1712  02367
      IF(ITH.EQ.0) GO TO 192                                    P1712  02368
C                                                               P1712  02369
C     SPECIAL THROAT INTERPOLATION IF ITH = 2                   P1712  02370
C                                                               P1712  02371
      DLNI = .5*TT*ENN/(HSUM(1)-HSUM(2))                        P1712  02372
      AA(ITH)=.5*DLNI*(2.*DLNI+(GAMMAS(2)-1.)/GAMMAS(2))        P1712  02373
      XX = ALOG(PCP(2))                                         P1712  02374
      BB(ITH) = 1./GAMMAS(2)-DLNI-2.*XX*AA(ITH)                 P1712  02375
      CC(ITH) = ENN*TT/(PP*(HSUM(1)-HSUM(2))**.5)               P1712  02376
      CC(ITH) = ALOG(CC(ITH))-XX*(BB(ITH)+AA(ITH)*XX)           P1712  02377
      IF(ITH.EQ.1)  GO TO 192                                   P1712  02378
      BB(1)=BB(1)-BB(2)                                         P1712  02379
      AA(1)=AA(1)-AA(2)                                         P1712  02380
      PCP(2)=(-BB(1)+(BB(1)*BB(1)-4.*AA(1)*(CC(1)-CC(2)))**.5)/(2.*AA(1) P1712  02381
     1)                                                         P1712  02382
      PCP(2)=EXP(PCP(2))                                        P1712  02383
      GO TO 193                                                 P1712  02384
  192 PCP(2)= PCP(2)/(1.+2.*DHSTAR/(ENN*TT *(GAMMAS(2)+1.)))    P1712  02385
  193 P(2) = P(1) / PCP(2)                                      P1712  02386
      PP = P(2)                                                 P1712  02387
      ITROT = ITROT-1                                           P1712  02388
      CALL COLBRM                                               P1712  02389
      IF(TT.EQ.0.) GO TO 1000                                   P1712  02390
      GO TO 190                                                 P1712  02391
C                                                               P1712  02392
  900 K = 0                                                     P1712  02393
      IF (.NOT.EQL .AND. FROZ) GO TO 990                        P1712  02394
      IF(IP.EQ.NP.OR.TT.EQ.0.)  GO TO 860                       P1712  02395
      K = NPT                                                   P1712  02396
      IF(NPT.NE.13)  GO TO 870                                  P1712  02397
  860 CALL RKTOUT                                               P1712  02398
      IFLGGG=1                                                  P1712  02399
      IF ((NSUB + NSUP).NE.0) CALL RATIO                        P1712  02400
      IF(K.EQ.0) GO TO 990                                      P1712  02401
      WRITE(6,865)                                              P1712  02402
  865 FORMAT(1H1)                                               P1712  02403
      NPT = 2                                                   P1712  02404
  870 NPT = NPT + 1                                             P1712  02405
C                                                               P1712  02406
C     SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT             P1712  02407
C                                                               P1712  02408
      DO 880 I = 1,NS                                           P1712  02409
      EN(I,NPT) = EN(I,K)                                       P1712  02410
  880 CONTINUE                                                  P1712  02411
  902 CONTINUE                                                  P1712  02412
  990 IF (FROZ) CALL FROZEN                                     P1712  02413
 1000 RETURN                                                    P1712  02414
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160          END                                                P1712   02415
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      SUBROUTINE SEARCH                                                P1712   02416
C                                                                      P1712   02417
C  SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED            P1712   02418
      INTEGER SUB,OMIT,ENL                                             P1712   02419
C                                                                      P1712   02420
      LOGICAL NEWR                                                     P1712   02421
C                                                                      P1712   02422
      DIMENSION DATE(2,3),MT(4),B(4),OMIT(3,3)                         P1712   02423
C                                                                      P1712   02424
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)  P1712   02425
     1 ,CELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)            P1712   02426
      COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),B0(15),BOP(15,2) P1712   02427
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBJ,AC(2),AM(2) P1712 02428
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)        P1712   02429
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712 02430
     4 ,RHOP,RMW(15),TLN,JANF                                          P1712   02431
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712 02432
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ    P1712   02433
     2 ,IONS,LC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                  P1712   02434
C                                                                      P1712   02435
      EQUIVALENCE (DATE,EN),(OMIT,ENLN),(ENDD,END)                     P1712   02436
C                                                                      P1712   02437
      DATA  GAS/1HG/,END/3HEND/                                        P1712   02438
C                                                                      P1712   02439
      NC= 0                                                            P1712   02440
      IX= 0                                                            P1712   02441
      COEF(1,1,1) = ENDD                                               P1712   02442
      DO 3 I=1,150                                                     P1712   02443
      ISAVE=I                                                          P1712   02444
      IF(A(1,I).EQ.ENDD)  GO TO 4                                      P1712   02445
      DO 3  J=1,L                                                      P1712   02446
      A(J,I) = 0.                                                      P1712   02447
    3 CONTINUE                                                         P1712   02448
    4 MAXNS=ISAVE                                                      P1712   02449
      REWIND 9                                                         P1712   02450
      READ (9,5) TLOW,THID,THIGH                                       P1712   02451
    5 FORMAT (3F10.3)                                                  P1712   02452
      NS = 1                                                           P1712   02453
    7 READ     (9,10)(SUB(NS,I),I=1,3),DATE(1,NS),DATE(2,NS),(MT(J),B(J), P1712 02454
     1  J=1,4),PHAZ,T1,T2                                              P1712   02455
   10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3)                          P1712   02456
      IF(SUB(NS,1).EQ.END) GO TO 171                                   P1712   02457
      READ (9,20)((COEF(I,J,NS),J=1,7),I=1,2)                          P1712   02458
   20 FORMAT (5E15.8)                                                  P1712   02459
      IF(NOMIT.EQ.0) GO TO 810                                         P1712   02460
      DO 805 I=1,NOMIT                                                 P1712   02461
      DO 804 J=1,3                                                     P1712   02462
      IF(OMIT(J,I).NE.SUB(NS,J)) GO TO 805                             P1712   02463
  804 CONTINUE                                                         P1712   02464
      GO TO 7                                                          P1712   02465
  805 CONTINUE                                                         P1712   02466
  810 DO 820 K=1,4                                                     P1712   02467
      IF(B(K).EQ.0.) GO TO 825                                         P1712   02468
```

```
              DO 168 I=1,L                                             P1712  02469
              IF(LLMT(I).EQ.MT(K)) GO TO 820                           P1712  02470
        168 CONTINUE                                                   P1712  02471
              DO 819 J=1,L                                             P1712  02472
        819 A(J,NS) = 0.                                               P1712  02473
              GO TO 7                                                  P1712  02474
        820 A(I,NS)= B(K)                                              P1712  02475
        825 IF(NS.EQ.MAXNS)  GO TO 870                                 P1712  02476
              IUSE(NS)= 0                                              P1712  02477
              IF(PHAZ.EQ.GAS) GO TO 170                                P1712  02478
              NC= NC+1                                                 P1712  02479
              TEMP(NC,1)= T1                                           P1712  02480
              TEMP(NC,2)= T2                                           P1712  02481
              IX= IX+1                                                 P1712  02482
              IF(IUSE(NS-1).EQ.0 .OR. NC.EQ.1) GO TO 145               P1712  02483
              DO 830 I=1,L                                             P1712  02484
              IF(A(I,NS).NE.A(I,NS-1)) GO TO 145                       P1712  02485
        830 CONTINUE                                                   P1712  02486
              IX= IX-1                                                 P1712  02487
        145 IUSE(NS)= -IX                                              P1712  02488
        170 NS= NS+1                                                   P1712  02489
              GO TO 7                                                  P1712  02490
        870 WRITE(6,871) (SUB(NS,J),J=1,3)                             P1712  02491
        871 FORMAT (45H0DIMENSICNS IN/SPECES/TOO SMALL TO CONSIDER ,3A4)  P1712  02492
              GO TO 7                                                  P1712  02493
        171 NS= NS-1                                                   P1712  02494
              NEWR= .FALSE.                                            P1712  02495
              WRITE(6,172)                                             P1712  02496
        172 FORMAT(42H0SPECIES BEING CONSIDERED IN THIS SYSTEM   )     P1712  02497
              DO 174 I=1,NS,5                                          P1712  02498
              I5= I+4                                                  P1712  02499
              IF(NS.LT.I5) I5=NS                                       P1712  02500
        174 WRITE (6,176)(DATE(1,J),DATE(2,J),SUB(J,1),SUB(J,2),SUB(J,3),J=I,  P1712  02501
           1  I5)                                                      P1712  02502
        176 FORMAT(5(5X,2A3,2X,3A4))                                   P1712  02503
              RETURN                                                   P1712  02504
              END                                                      P1712  02505
```

```
      SUBROUTINE SET(ONE,TWO,THREE,ARG,HAL)                             P1712  02506
C                                                                       P1712  02507
C     (USED FOR AREA RATIO INTERPOLATION ONLY)                          P1712  02508
C     SETS UP ALL 4 BY 5 MATRICES                                       P1712  02509
C                                                                       P1712  02510
C     DOUBLE PRECISION A,ANS,G,X                                        P1712  02511
C                                                                       P1712  02512
      DIMENSION ANS(6),ONE(2),TWO(2),THREE(2),A(20,21)                  P1712  02513
C                                                                       P1712  02514
      COMMON/DOUBLE/G(20,21),X(20)                                      P1712  02515
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS,P1712  02516
     1 KMAT,IMAT,IG1,N,J,NOMIT,IF,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ      P1712  02517
     2 ,IONS,NO,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                   P1712  02518
C                                                                       P1712  02519
      EQUIVALENCE (G,A),(X,ANS)                                         P1712  02520
C                                                                       P1712  02521
      DO 8 J=1,2                                                        P1712  02522
      A(J,5)=ALOG(ONE(J))                                               P1712  02523
      A(J+2,5)=TWO(J)                                                   P1712  02524
      A(J,2)=ALOG(THREE(J))                                             P1712  02525
    8 CONTINUE                                                          P1712  02526
      DO 1 I=1,2                                                        P1712  02527
      A(I,1)=1.0                                                        P1712  02528
      A(I+2,1)=0.0                                                      P1712  02529
      A(I+2,2)=1.0                                                      P1712  02530
      DO 1 J=2,3                                                        P1712  02531
      A(I,J+1)=A(I,2)**J                                                P1712  02532
      MXP=J-1                                                           P1712  02533
      A(I+2,J+1)=A(I,2)**MXP*FLOAT(J)                                   P1712  02534
    1 CONTINUE                                                          P1712  02535
      IMAT = 4                                                          P1712  02536
      CALL MGAUSD                                                       P1712  02537
      HAL=ANS(1)                                                        P1712  02538
      SUM=ALOG(ARG)                                                     P1712  02539
      DO 10 J=1,3                                                       P1712  02540
      HAL=HAL+SUM**J*(ANS(J+1))                                         P1712  02541
   10 CONTINUE                                                          P1712  02542
      HAL=EXP(HAL)                                                      P1712  02543
      RETURN                                                            P1712  02544
      END                                                               P1712  02545
```

```
      SUBROUTINE VISCON(NS,NPT,SUB,EN,TOTN,T)                           P171201 00010
C                                                                       P171201 00011
C   THIS SUBROUTINE COMPUTES THE VISCOSITY AND THE CONDUCTIVITY         P171201 00012
C   OF A GAS MIXTURE CONSISTING OF 5 GASEOUS SPECIES.                   P171201 00013
C   GASEOUS SPECIES TO BE CONSIDERED ARE H2O,CO,H2,CO2,AND N2.          P171201 00014
C                                                                       P171201 00015
      COMMON/PRCENT/ FMOLE                                              P171201 00016
      DIMENSION SUB(150,3),EN(150,13),TOTN(13),T(13),SPECE(5),EK(5),    P171201 00017
     1SIG(5),WGTM(5),TE(33),OMEG(33),FMOLE(5),VIS(5),COND(5),           P171201 00018
     2VISMIX(13),CONMIX(13)                                             P171201 00019
      DATA (SPECE(I),I=1,5)/4HH2O ,4HCO  ,4HH2  ,4HCO2 ,4HN2  /         P171201 00020
      DATA (SIG(I),I=1,5)/2.824,3.706,2.915,3.897,3.749/                P171201 00021
      DATA (EK(I),I=1,5)/230.9,85.0,38.0,213.0,79.8/                    P171201 00022
      DATA (WGTM(I),I=1,5)/18.,28.01,2.016,44.01,28.02/                 P171201 00023
      DATA CON1,CON2,CONS/ 0.000026693,0.00019891,0.35355339059/        P171201 00024
      DATA (TE(I),I=1,33)/1.0,1.2,1.4,1.6,1.8,2.0,2.2,2.4,2.6,2.8,3.0,  P171201 00025
     13.2,3.4,3.6,3.8,4.0,5.0,6.0,7.0,8.0,9.0,10.0,11.0,12.0,13.0,14.0, P171201 00026
     215.0,16.0,32.0,64.0,128.0,256.0,512.0/                            P171201 00027
      DATA (OMEG(I),I=1,33)/1.5938,1.4568,1.3557,1.2900,1.2216,1.1791,  P171201 00028
     11.1377,1.1066,1.0803,1.0579,1.0385,1.0214,1.0063,0.9928,0.9807,   P171201 00029
     20.9696,0.9265,0.8960,0.8725,0.8536,0.8378,0.8242,0.8123,0.8017,   P171201 00030
     30.7922,0.7836,0.7756,0.7883,0.6939,0.6262,0.5634,0.5056,0.4528/   P171201 00031
C                                                                       P171201 00032
C   VALUES FOR VISCOSITY AND CONDUCTIVITY WILL BE COMPUTED AT THE       P171201 00033
C   CHAMBER,THE THROAT,AND AT THE ASSIGNED EXITS.                       P171201 00034
C                                                                       P171201 00035
C     WRITE(6,8999) NS,NPT                                              P171201 00036
 8999 FORMAT(2I10)                                                      P171201 00037
      PMOLE=0.0                                                         P171201 00038
         DO 1000 M=1,NPT                                                P171201 00039
C                                                                       P171201 00040
C   COMPUTE THE MOLE FRACTIONS OF THE 5 GASEOUS SPECIES.                P171201 00041
C                                                                       P171201 00042
      DO 20 I=1,5                                                       P171201 00043
      DO 10 J=1,NS                                                      P171201 00044
C                                                                       P171201 00045
C   SEARCH THE ARRAY SUB(J,1) FOR THE 5 NEEDED SPECIES. WHEN ONE OF THE P171201 00046
C   NEEDED SPECIES IS FOUND,COMPUTE THE MOLE FRACTION.                  P171201 00047
C                                                                       P171201 00048
      IF(SPECF(I).NE.SUB(J,1)) GO TO 10                                 P171201 00049
      FMOLE(I)=EN(J,M)/TOTN(M)                                          P171201 00050
C     WRITE(6,9000) SPECE(I),SUB(J,1),EN(J,M),TOTN(M),FMOLE(I),I,J,M    P171201 00051
 9000 FORMAT(1X,2A10,3F15.8,3I5)                                        P171201 00052
      IF(M.EQ.1) PMOLE=PMOLE+FMOLE(I)*100.                              P171201 00053
      GO TO 20                                                          P171201 00054
   10 CONTINUE                                                          P171201 00055
C   IF THE SPECIE CANNOT BE LOCATED IN THE ARRAY SUB(J,1), SET THE MOLE P171201 00056
C   FRACTION TO MINUS ONE.                                              P171201 00057
C                                                                       P171201 00058
      FMOLE(I)=-1.0                                                     P171201 00059
   20 CONTINUE                                                          P171201 00060
C                                                                       P171201 00061
C   COMPUTE THE VISCOSITY AND THE CONDUCTIVITY FOR EACH OF THE 5 SPECIES P171201 00062
```

```
      C                                                               P171201 00063
            DO 100 I=1,5                                              P171201 00064
            IF(FMOLE(I).LT.0.0) GO TO 100                             P171201 00065
            TEK=T(M)/EK(I)                                            P171201 00066
            IF(TEK.LT.TE(1)) TEK=TE(1)                                P171201 00067
            IF(TEK.GT.TE(33)) TEK=TE(33)                              P171201 00068
            DO 40 J=1,33                                              P171201 00069
            IF(TEK-TE(J)) 30,25,40                                    P171201 00070
         25 DOM=OMEG(J)                                               P171201 00071
            GO TO 50                                                  P171201 00072
         30 FRAC=(TEK-TE(J-1))/(TE(J-1)-TE(J))                        P171201 00073
            DOM=OMEG(J-1)+FRAC*(OMEG(J-1)-OMEG(J))                    P171201 00074
            GO TO 50                                                  P171201 00075
         40 CONTINUE                                                  P171201 00076
         50 DIV=SIG(I)*SIG(I)*DOM                                     P171201 00077
      C                                                               P171201 00078
      C   VISCOSITY                                                   P171201 00079
      C                                                               P171201 00080
            VIS(I)=CON1*SQRT(WGTM(I)*T(M))/DIV                        P171201 00081
      C                                                               P171201 00082
      C   CONDUCTIVITY                                                P171201 00083
      C                                                               P171201 00084
            COND(I)=CON2*SQRT(T(M)/WGTM(I))/DIV                       P171201 00085
      C     WRITE(6,9001) T(M),EK(I),TEK,TE(J-1),TE(J),FRAC,OMEG(J-1),OMEG(J), P171201 00086
      C    1DIV,DOM,SIG(I),WGTM(I),VIS(I),COND(I),I,J,M               P171201 00087
       9001 FORMAT(8F15.8,/6F15.8,3I5)                                P171201 00088
        100 CONTINUE                                                  P171201 00089
      C                                                               P171201 00090
      C   COMPUTE VISCOSITY AND CONDUCTIVITY OF MIXTURE.              P171201 00091
      C                                                               P171201 00092
            VISMIX(M)=0.0                                             P171201 00093
            CONMIX(M)=0.0                                             P171201 00094
            DO 200 I=1,5                                              P171201 00095
            SUM=0.0                                                   P171201 00096
            IF(FMOLE(I).LT.0.0) GO TO 200                             P171201 00097
            DO 150 J=1,5                                              P171201 00098
            IF(FMOLE(J).LT.0.0) GO TO 150                             P171201 00099
            F1=SQRT(1.+WGTM(I)/WGTM(J))                               P171201 00100
            F2=SQRT(VIS(I)/VIS(J))                                    P171201 00101
            F3=(WGTM(J)/WGTM(I))**(0.25)                              P171201 00102
            FA=1.+F2*F3                                               P171201 00103
            FAC=CONS/F1                                               P171201 00104
            PHI=FAC*FA*FA                                             P171201 00105
            SUM=SUM+FMOLE(J)*PHI                                      P171201 00106
      C     WRITE(6,9002) FMOLE(I),FMOLE(J),WGTM(I),WGTM(J),F1,VIS(I),VIS(J), P171201 00107
      C    1F2,COND(I),COND(J),F3,FA,FAC,PHI,SUM,I,J,M                P171201 00108
       9002 FORMAT(8F15.8/7F15.8,3I5)                                 P171201 00109
        150 CONTINUE                                                  P171201 00110
      C                                                               P171201 00111
      C   VISCOSITY OF MIXTURE                                        P171201 00112
      C                                                               P171201 00113
            VISMIX(M)=VISMIX(M)+FMOLE(I)*VIS(I)/SUM                   P171201 00114
      C                                                               P171201 00115
```

```
      C     CONDUCTIVITY OF MIXTURE                          P171201 00116
      C                                                      P171201 00117
            CONMIX(M)=CONMIX(M)+FMOLE(I)*COND(I)/SUM         P171201 00118
      C     WRITE(6,9009) VISMIX(M),CONMIX(M),M              P171201 00119
       9009 FORMAT(1X,2F15.11,3X,I5)                         P171201 00120
        200 CONTINUE                                         P171201 00121
       1000 CONTINUE                                         P171201 00122
            WRITE(6,2000) (VISMIX(I),I=1,NPT)                P171201 00123
            WRITE(6,2100) (CONMIX(I),I=1,NPT)                P171201 00124
       2000 FORMAT(1H ,*VISC, G/CM-SEC*,13F9.6)              P171201 00125
       2100 FORMAT(1H ,*C, CAL/G-SEC-K*,13F9.6)              P171201 00126
            RETURN                                           P171201 00127
            END                                              P171201 00128
```


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APPENDIX II

POLYNOMIAL FIT PROGRAM

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```
      PROGRAM SLSQF(INPUT,OUTPUT)
      DIMENSION TT(100),CPR(100),HTR(100),STR(100)
      DIMENSION CCPR(100),CHTR(100),CSTR(100)
      DIMENSION NPT(2),NAME(6)
      COMMON/MATRIX/ G(10,11),X(10),IMAT
      R=1.98726
      ASSIGN 500 TO MEOF
      IF(EOF(MEOF)) 500,500,1
    1 READ 40,HO,NPT,NAME
   40 FORMAT(F10.1,2I3,4X,6A10)
      PRINT 112,NAME,HO
  112 FORMAT((1H1,29X,6A10//1P,5HHO = ,F10.1//)
      KPT=0
  111 KPT=KPT+1
      NVAL=NPT(KPT)
      READ 6,(TT(K),K=1,NVAL)
      READ 7,(CPR(K),K=1,NVAL)
      READ 7,(HTR(K),K=1,NVAL)
      DO 22 I=1,NVAL
   22 HTR(I)=HTR(I)*1000.+HO
      READ 7,(STR(K),K=1,NVAL)
    6 FORMAT(20F4.0)
    7 FORMAT(10F8.3)
      DO 16 I=1,10
      DO 15 J=1,11
      G(I,J)=0.
   15 CONTINUE
   16 CONTINUE
      SUMT=0.
      SUMT2=0.
      SUMT3=0.
      SUMT4=0.
      SUMT5=0.
      SUMT6=0.
      SUMT7=0.
      SUMT8=0.
      SUMTM2=0.
      DO 100 K=1,NVAL
      T=TT(K)
      CP=CPR(K)/R
      HT=HTR(K)/(R*T)
      ST=STR(K)/R
      TLOG=ALOG(T)
      T2=T**2
      T3=T2*T
      T4=T3*T
      T5=T4*T
      T6=T5*T
      T7=T6*T
      T8=T7*T
      TREC=1.0/T
      TM2=1.0/T2
      SUMT=SUMT+T
```

```
      SUMT2=SUMT2+T2
      SUMT3=SUMT3+T3
      SUMT4=SUMT4+T4
      SUMT5=SUMT5+T5
      SUMT6=SUMT6+T6
      SUMT7=SUMT7+T7
      SUMT8=SUMT8+T8
      SUMTM2=SUMTM2+TM2
      G(1,1)=G(1,1)+2.+TLOG**2
      G(1,2)=G(1,2)+(1.5+TLOG)*T
      G(1,3)=G(1,3)+(4./3.+.5*TLOG)*T2
      G(1,4)=G(1,4)+(1.25+TLOG/3.)*T3
      G(1,5)=G(1,5)+(1.2+TLOG/4.)*T4
      G(1,6)=G(1,6)+TREC
      G(1,7)=G(1,7)+TLOG
      G(1,11)=G(1,11)+CP+HT+ST*TLOG
      G(2,11)=G(2,11)+(CP+.5*HT+ST)*T
      G(3,11)=G(3,11)+(CP+HT/3.+.5*ST)*T2
      G(4,11)=G(4,11)+(CP+HT/4.+ST/3.)*T3
      G(5,11)=G(5,11)+(CP+HT/5.+ST/4.)*T4
      G(6,11)=G(6,11)+HT*TREC
      G(7,11)=G(7,11)+ST
      IF(K.GT.1) GO TO 50
      G(1,8)=1.0
      G(1,9)=1.0
      G(1,10)=TLOG
      G(2,6)=FLOAT(NVAL)/2.0
      G(2,8)=T
      G(2,9)=T/2.0
      G(2,10)=T
      G(3,8)=T2
      G(3,9)=T2/3.
      G(3,10)=T2/2.
      G(4,8)=T3
      G(4,9)=T3/4.
      G(4,10)=T3/3.
      G(5,8)=T4
      G(5,9)=T4/5.
      G(5,10)=T4/4.
      G(6,9)=TREC
      G(7,7)=FLOAT(NVAL)
      G(7,10)=1.0
      G(8,11)=CP
      G(9,11)=HT
      G(10,11)=ST
   50 CONTINUE
  100 CONTINUE
      G(2,2)=(9./4.)*SUMT2
      G(2,3)=(5./3.)*SUMT3
      G(2,4)=(35./24.)*SUMT4
      G(2,5)=(27./20.)*SUMT5
      G(2,7)=SUMT
      G(3,3)=(49./36.)*SUMT4
```

```
      G(3,4)=(5./4.)*SUMT5
      G(3,5)=(143./120.)*SUMT6
      G(3,6)=SUMT/3.
      G(3,7)=SUMT2/2.
      G(4,4)=(169./144.)*SUMT6
      G(4,5)=(17./15.)*SUMT7
      G(4,6)=SUMT2/4.
      G(4,7)=SUMT3/3.
      G(5,5)=(441./400.)*SUMT8
      G(5,6)=SUMT3/5.
      G(5,7)=SUMT4/4.
      G(6,6)=SUMTM2
      DO 200 I=1,10
      DO 210 J=I,10
      IF(I.EQ.J) GO TO 210
      G(J,I)=G(I,J)
  210 CONTINUE
  200 CONTINUE
      PRINT 92
      IF(DEBUG(1).NE.0.0) GO TO 190
   92 FORMAT(1H ,*VALUES OF G*)
      DO 90 I=1,10
      PRINT 91,(G(I,J),J=1,11)
   91 FORMAT(1X,11E11.5)
   90 CONTINUE
  190 IMAT=10
      CALL MGAUSD
      PRINT 94
   94 FORMAT(1H ,*COEFFICIENTS ARE*)
      PRINT 192,X
  192 FORMAT(1X,7E15.8/1X,3E15.8)
      DO 400 I=1,NVAL
      T=TT(I)
      T2=T*T
      T3=T2*T
      T4=T3*T
      TLOG=ALOG(T)
      CCPR(I)=X(1)+X(2)*T+X(3)*T2+X(4)*T3+X(5)*T4
      CCPR(I)=CCPR(I)*R
      CHTR(I)=((X(1)+X(2)*T/2.+X(3)*T2/3.+X(4)*T3/4.+X(5)*T4/5.)*T+X(6))
     1*R
      CHTR(I)=(CHTR(I)-HO)/1000.
      CSTR(I)=(X(1)*TLOG+X(2)*T+X(3)*T2/2.+X(4)*T3/3.+X(5)*T4/4.+X(7)
     1R
  400 CONTINUE
      PRINT 401
  401 FORMAT(1H ,*    T         CP       CCP        HT       CHT       ST       CST
     1      DCP      DHT      DST*//)
      DO 410 I=1,NVAL
      DCPR=ABS(CPR(I)-CCPR(I))
      DTR=(HTR(I)-HO)/1000.
      DHTS=ABS(DTR-CHTR(I))
      DSTR=ABS(STR(I)-CSTR(I))
```

```
 411 FORMAT(1H ,1X,F5.0,9F8.3)
     PRINT 411,TT(I),CPR(I),CCPR(I),DTR,CHTR(I),STR(I),CSTR(I),DCPR,
    1CHTR,DSTR
 410 CONTINUE
     GO TO (111,1),KPT
 500 CONTINUE
     END
```

```
          SUBROUTINE MGAUSD
C
C         SOLVE AN( LINEAR SET OF UP TO 20 EQUATIONS
C
C         DOUBLE PRECISION G,X,COEFX(20),SUM,Z
          DIMENSION COEFX(20)
C
          COMMON/MATRIX/ G(10,11),X(10),IMAT
C
          EQUIVALENCE (IUSE,IMAT)
C
C         DATA BIGNO/1.E+38/
          DATA BIGNO/1.E+320/
C
C         BEGIN ELIMINATION OF NNTH VARIABLE
C
          IUSE1=IUSE+1
        6 DO 45 NN=1,IUSE
          IF (NN-IUSE) 8,83,8
       83 IF(G(NN,NN))31,23,31
C
C         SEARCH FO  AXIMUM COEFFICIENT IN EACH ROW
C
        8 DO 18 I=NN,IUSE
          COEFX(I) = BIGNO
          IF(G(I,NN).EQ.0.)  GO TO 18
          COEFX(I) = 0.
          DO 10 J=NN,IUSE1
          SUM = G(I,J)
          IF(SUM.LT.0.)  SUM=-SUM
          IF(J.NE.NN)  GO TO 9
          Z = SUM
          GO TO 10
        9 IF(SUM.GT.COEFX(I))  COEFX(I)=SUM
       10 CONTINUE
          COEFX(I) = COEFX(I)/Z
       18 CONTINUE
          TEMP = BIGNO
          I=0
       20 DO 22 J=NN,IUSE
          IF (COEFX(J)-TEMP) 87,22,22
       87 TEMP=COEFX(J)
          I=J
       22 CONTINUE
          IF(I) 28,23,28
C
C         INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH
C         VARIABLE FROM THE REMAINING EQUATIONS
C
C          INTERCHANGE EQUATIONS I AND NN
C
       28 IF(NN-1) 29,31,29
       29 DO 30 J=NN,IUSE1
```

```
          Z=G(I,J)
          G(I,J)=G(NN,J)
          G(NN,J)=Z
   30 CONTINUE
C
C     DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH
C     VARIABLE FROM THE REMAINING EQUATIONS
C
   31 K = NN + 1
      DO 36 J = K, IUSE1
      IF((NN,NN).EQ.0.)  GO TO 23
          G(NN,J) = G(NN,J) / G(NN,NN)
   36 CONTINUE
      IF(K-IUSE1) 88,45,88
   88 DC 44 I = K,IUSE
   40 DO 44 J = K, IUSE1
          G(I,J) = G(I,J) - G(I,NN)*G(NN,J)
   44 CONTINUE
   45 CONTINUE
C
C     BACKSOLVE FOR THE VARIABLES
C
      K = IUSE
   47 J = K + 1
C     X(K) = 0.0D0
      X(K) = 0.0
      SUM = 0.0
      IF(IUSE - J) 51,48,46
   48 DC 50 I = J,IUSE
          SUM = SUM + G(K,I)* X(I)
   50 CONTINUE
   51 X(K) = G(K,IUSE1) - SUM
      K = K - 1
      IF (K) 47,151,47
   23 IUSE = IUSE-1
  151 RETURN
      END
```

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